

DFT		pyscf	cp2k		single cyc	max pyscf time	max cp2k time		highest 3 pyscf	lowest 3 pyscf	mean highest	mean lowest		highest 3 cp2k	lowest 3 cp2k	mean highest	mean lowest
System Si Diamond	Functional:	lda	lda			42.88 sec	2.4 sec		44.28	4.6	33.56333333	8.49		4.7	1.9	4.53333333	2.73333333
	Basis:	dzvp	dzvp						42.88	4.52				4.7	2.8		
	Energy:	-31.28980517	-31.29788527						13.53	16.35				4.2	3.5		
	Time (sec)	1129.372854	23.024	49.05198289													
	homo-lumo gap (a.u)	0.00996907422	0.01744552943														
Diamond	Functional:	lda	lda			42.85 sec	2.4 sec		42.81	9	35.78	13.23		2.1	0.9	2.03333333	1.5
	Basis:	dzvp	dzvp						42.85	8.42				2	1.8		
	Energy:	-45.10667858	-45.08874225						21.68	22.27				2	1.8		
	Time (sec)	87.48938298	26.249	3.333055849													
	homo-lumo gap (a.u)	0.1544400057	0.1640567053														
LiH	Functional:	lda	lda			27.49 sec	2.9 sec		27.17	3.96	27.37333333	8.4		5.6	2.2	5.73333333	3.7
	Basis:	dzvp	dzvp						27.46	4				5.7	4.3		
	Energy:	-7.898788585	-7.899728236						27.49	17.24				5.9	4.6		
	Time (sec)	433.965961	138.2291181	3.139468492													
	homo-lumo gap (a.u)	0.1526107681	0.151307066														
LiF	Functional:	lda	lda			95.21 sec	3 sec										
	Basis:	dzvp	dzvp														
	Energy:	-31.50423604	-31.52945473						95.21	12.94	92.59333333	22.65333333		3	1.2	3	1.93333333
	Time (sec)	51.324	33.99907994	1.509570262					95.62	13.1				3	2.3		
	homo-lumo gap (a.u)	0	0.0683704659						86.95	41.92				3	2.3		
LiCl	Functional:	lda	lda														
	Basis:	dzvp	dzvp			30.44 sec	2.7 sec		30.44	2.83	31.36333333	6.25333333		8.7	1.4	6.2	2.23333333
	Energy:	-22.32183456	-22.32453313						33.27	3.11				4.8	2.6		
	Time (sec)	196.3624921	35.479	5.534611801					30.38	12.82				5.1	2.7		
	homo-lumo gap (a.u)	0	0.06168352193														
MgO	Functional:	lda	lda														
	Basis:	dzvp	dzvp						113.92	8.1	98.86	43.49333333		6	0.8	7	1.33333333
	Energy:	-78.75057618	-78.82991817						91.34	31.06				6.6	1.6		
	Time (sec)	982.7888191	457.59	2.147749774		113.92 sec	1.4 sec		91.32	91.32				8.4	1.6		
	homo-lumo gap (a.u)	0	0.000165739456														
Ge	Functional:	lda	lda														
	Basis:	dzvp	dzvp														
	Energy:	-7.630077435	-7.643054214														
	Time (sec)	135.684011	34.521	3.930477419		18.11 sec	2.4 sec		17.15	0.61	16.11	3.396666667		5.6	0.7	5.33333333	1.73333333
	homo-lumo gap (a.u)	0.00491107256	1.90E-05						18.11	2.55				5.3	2.2		
									13.07	7.03				5.1	2.3		
SiC	Functional:	lda	lda														
	Basis:	dzvp	dzvp														
	Energy:	-9.151123291	-9.158338311														
	Time (sec)	271.8020539	71.359	3.808938661		60.83 sec	2.4 sec		49.66	1.01	49.33	9.413333333		4.4	1.1	4.266666667	1.566666667
	homo-lumo gap (a.u)	0.1075686123	smearing						37.5	22.49				4.1	1.8		
									60.83	4.74							
BN	Functional:	lda	lda														
	Basis:	dzvp	dzvp														
	Energy:	-12.26747382	-12.28736725						57.63	1.07	47.19	11.41666667		1.9	0.3	1.866666667	0.533333333
	Time (sec)	254.463897	78.341	3.248157376		59.46 sec	2.1 sec		59.46	16.59				1.9	0.6		
	homo-lumo gap (a.u)	0.003709834767	had to use smearing to converge? questionable.						24.48	16.59				1.8	0.7		
AIP	Functional:	lda	lda														
	Basis:	dzvp	dzvp														
	Energy:	-8.398916597	-8.416939879						17.26	0.39	13.94666667	1.646666667		14	1.3	13.33333333	3
	Time (sec)	92.39292717	171.787	0.5378342201		17.26 sec	5.9 sec		12.81	2.79				13.5	3.1		
	homo-lumo gap (a.u)	0.002936977675	smearing						11.77	1.76				12.5	4.6		
ZnS	Functional:	lda	lda														
	Basis:	dzvp	dzvp														

	Energy:	-70.44524994	-70.46667894					218.92	6.73	155.8833333	14.88			20.6	2.5	18.26666667	3.833333333
	Time (sec)	554.0053611	222.405	2.490975298		216.97 sec	6.4 sec	31.76	6.69					19	4.3		
	homo-lumo gap (a.u)	0.1293346357	smearing					216.97	31.22					15.2	4.7		
GaAs	Functional:	lda	lda														
	Basis:	dzvp	dzvp														
	Energy:	-80.62453781	-80.62508416					250.66	97.74	284.2466667	46.66333333			31.5	4.2	31.06666667	5.1
	Time (sec)	2490.429532	242.144	10.28491118		322.09 sec	8.6 sec	322.09	7.42					30.2	5.4		
	homo-lumo gap (a.u)	0.05780635655	smearing					279.99	34.83					31.5	5.7		
GaN	Functional:	lda	lda														
	Basis:	dzvp	dzvp					160.82	26.03	158.5833333	36.48333333			15.1	1.6	11.83333333	2.633333333
	Energy:	-84.1080051	-84.11181043					144.82	5.63					10.3	3.1		
	Time (sec)	1389.231176	85.643	16.22118768		120.11 sec	4.5 sec	170.11	77.79					10.1	3.2		
	homo-lumo gap (a.u)	0.003036608856	smearing														
ZnO	Functional:	lda	lda														
	Basis:	dzvp	dzvp					1377.49	21.63	1217.233333	246.6333333			6.9	1.3	6.9	1.933333333
	Energy:	-152.3815636	-152.3500246					1189.9	368.61					6.9	2		
	Time (sec)	26289.7659	510.218	51.52653553		1377.49 sec	34.3 sec	1084.31	349.66					6.9	2.5		
	homo-lumo gap (a.u)	0.1453590745	smearing														
CdS	Functional:	lda	lda														
	Basis:	dzvp	dzvp														
	Energy:	-56.0492658	-56.07936939					62.43	1.83	39.35333333	14.27333333			23.6	2.6	24	5.466666667
	Time (sec)	2037.210173	450.688	4.5202228		65.43 sec	15.3 sec	32.68	18.08					24.7	6.7		
	homo-lumo gap (a.u)	0.1797310264	smearing					22.95	22.91					23.7	7.1		