

DFT		pyscf	cp2k		
System	Functional:	lda	lda		
Si Diamond	Basis:	dzvp	dzvp		
	Energy:	-31.28980517	-31.29788527		
	Time (sec)	1129.372854	23.024		
	homo-lumo gap (a.u)	0.00996907422	0.01744552943		
Diamond	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-45.10667858	-45.08874225		
	Time (sec)	87.48938298	26.249		
	homo-lumo gap (a.u)	0.1544400057	0.1640567053		
LiH	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-7.898788585	-7.899728236		
	Time (sec)	433.965961	138.2291181		
	homo-lumo gap (a.u)	0.1526107681	0.151307066		
LiF	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-31.50423604	-31.52945473		
	Time (sec)	51.324	33.99907994		
	homo-lumo gap (a.u)	0	0.0683704659		
LiCl	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-22.32183456	-22.32453313		
	Time (sec)	196.3624921	35.479		
	homo-lumo gap (a.u)	0	0.06168352193		

MgO	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-78.75057618	-78.82991817		
	Time (sec)	982.7888191	457.59		
	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		
	homo-lumo gap (a.u)	0.00491107256	1.90E-05		
SiC	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-9.151123291	-9.158338311		
	Time (sec)	271.8020539	71.359		
	homo-lumo gap (a.u)	0.1075686123	smearing		
BN	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-12.26747382	-12.28736725		
	Time (sec)	254.463897	78.341		
	homo-lumo gap (a.u)	0.003709834767	had to use smearing to converge? questionable.		
AIP	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-8.398916597	-8.416939879		
	Time (sec)	92.39292717	171.787		
	homo-lumo gap (a.u)	0.002936977675	smearing		

ZnS	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-70.44524994	-70.46667894		
	Time (sec)	554.0053611	222.405		
	homo-lumo gap (a.u)	0.1293346357	smearing		
GaAs	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-80.62453781	-80.62508416		
	Time (sec)	2490.429532	242.144		
	homo-lumo gap (a.u)	0.05780635655	smearing		
GaN	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-84.1080051	-84.11181043		
	Time (sec)	1389.231176	85.643		
	homo-lumo gap (a.u)	0.003036608856	smearing		
ZnO	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-152.3815636	-152.3500246		
	Time (sec)	26289.7659	510.218		
	homo-lumo gap (a.u)	0.1453590745	smearing		
CdS	Functional:	lda	lda		
	Basis:	dzvp	dzvp		
	Energy:	-56.0492658	-56.07936939		
	Time (sec)	2037.210173	450.688		
	homo-lumo gap (a.u)	0.1797310264	smearing		