Supporting information for: Resolution of the Band Gap Prediction Problem for Materials Design

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1 Basis Set Recipe

Our basis sets were chosen according to the following systematic recipe:

- For elements up to chlorine, we chose 6-311++G** by default. Because very diffuse basis functions can cause linear dependence in basis sets, basis functions were removed so that there was only one basis function with an exponent less than 0.1. We only retain the basis function with the largest exponent less than 0.1. All basis functions with smaller exponents are removed.

- If this modified basis could be used without numerical (linear dependence) problems, we used it. Otherwise, we replaced the most diffuse exponent with 0.1.

- If this modified basis could be used without numerical (linear dependence) problems, we used it. Otherwise, we replaced the most diffuse exponent with 0.12.

- If this modified basis could be used without numerical (linear dependence) problems, we used it. Otherwise, this basis function was removed.

In several cases, the above procedure did not yield a linearly independent basis set. Thus, we made the following modifications.

- For oxygen, we used the 6-31d1 basis set of Gatti et al.[S1]

- For LiF, we removed all basis functions with exponents below 0.1 from the aug-cc-PCVTZ basis set.

- For Co, Ni, and Mn, we used 6-31G* and followed the above procedure for treating diffuse exponents.

- We used 6-31G for Fe and followed the above procedure for treating diffuse exponents.

- For all SiC polymorphs, we used 6-31+G** for Si and followed the above procedure for treating diffuse exponents.

- For AlN (zincblende and wurtzite), AlP, AlAs, and AlSb, we used 6-31+G** for Al and followed the above procedure for treating diffuse exponents.

For Sr and all elements from Cu to Bi, we used Stuttgart fully relativistic pseudopotentials and the accompanying cc-PVDZ-level basis sets with the same treatment of diffuse exponents outlined above.

2 Comparison of B3PW and G_0W_0

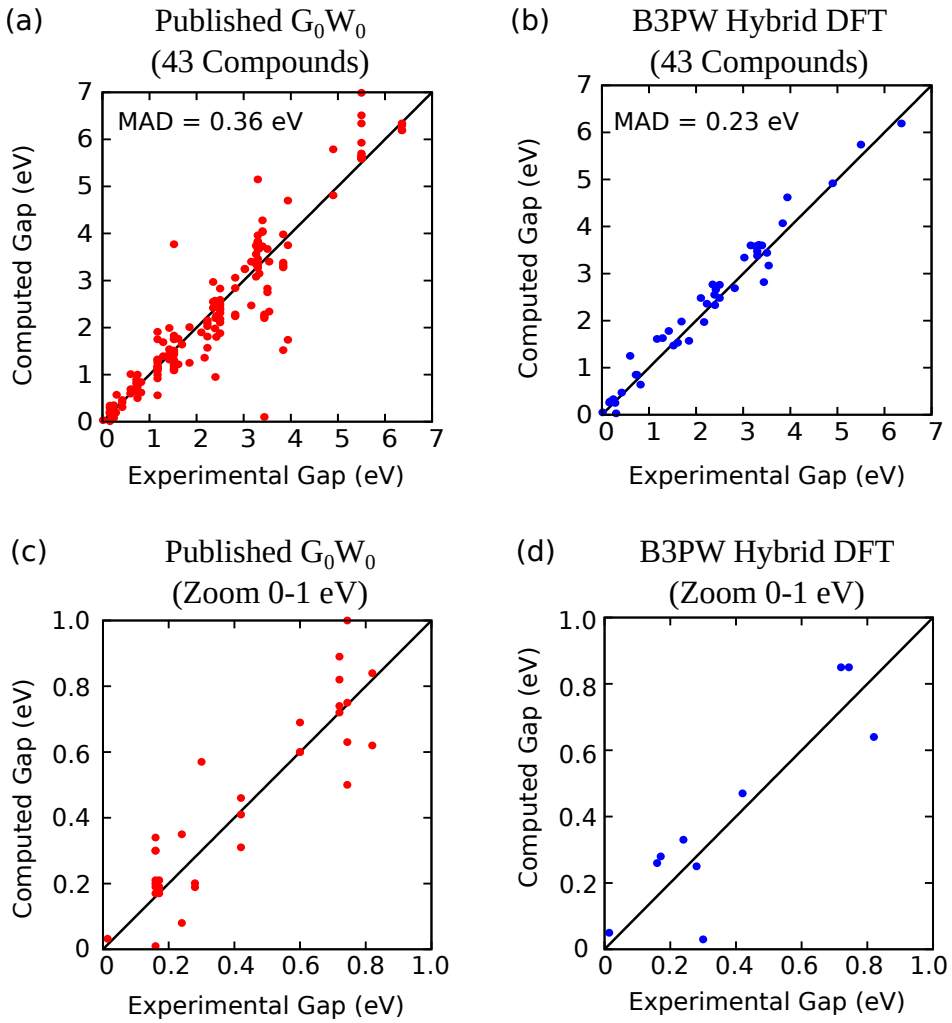

Figure S1: G_0W_0 and B3PW calculated band gaps versus experiment (low-temperature) for 43 compounds with band gaps below 7 eV. These 43 compounds are those for which our literature search found G_0W_0 results, and are a subset of the 70 compounds listed in Figures 2 and 3. These 43 compounds are listed in Figure S2. (a) Published G_0W_0 results (164 data points, 43 compounds, 32 publications). The mean absolute deviation (MAD) is 0.36 eV. (b) B3PW hybrid DFT calculations on the same 43 compounds. The MAD is 0.23 eV. (c) Zoom of (a) from 0–1 eV. (d) Zoom of (b) from 0–1 eV.

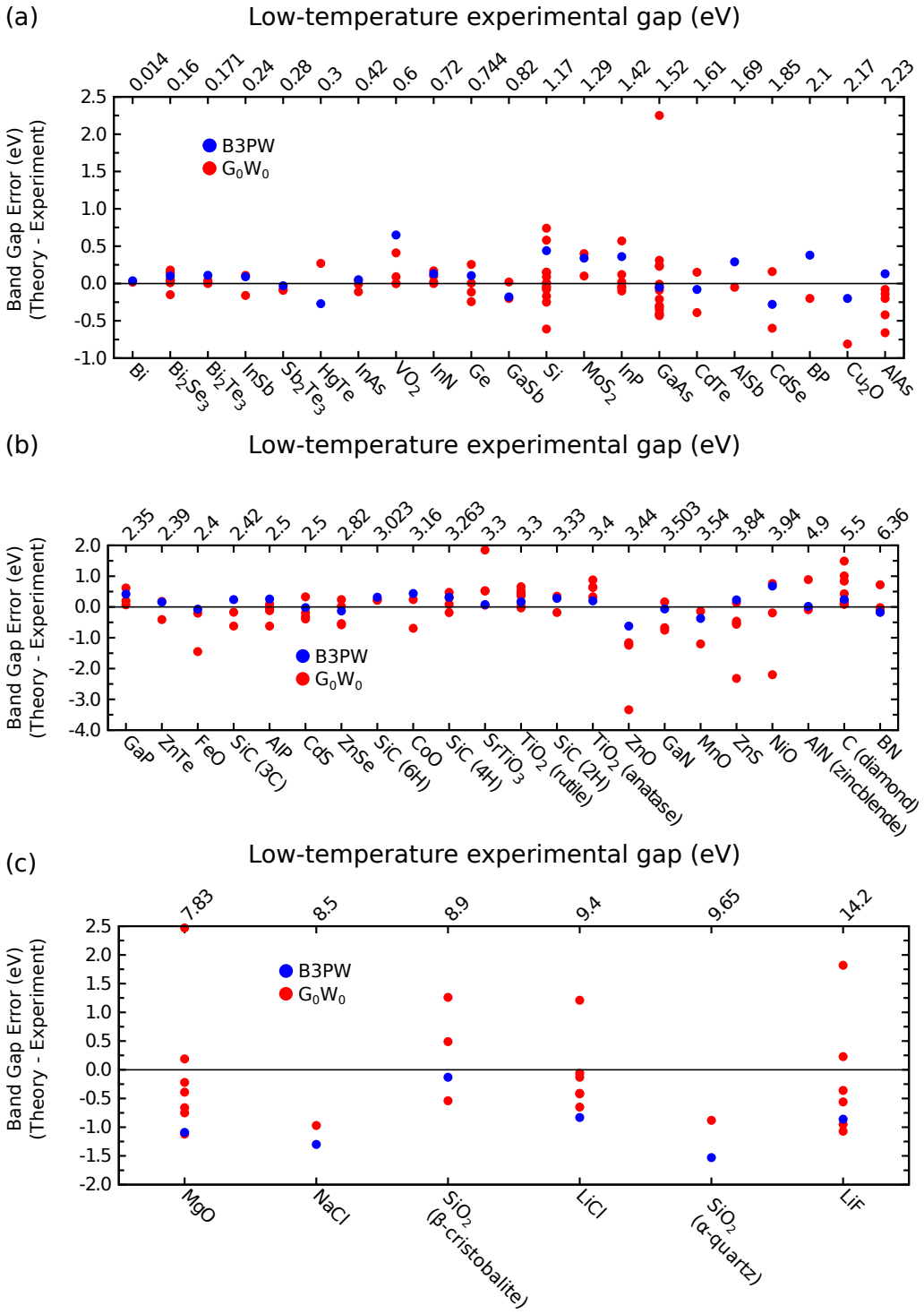

Figure S2: Difference between computed and low-temperature experimental band gaps for the 49 compounds for which our literature search found G_0W_0 results. Our B3PW results are shown by blue circles, and red circles represent literature G_0W_0 results. Compound names are listed on the bottom x-axes; experimental band gaps (low temperature or $T \approx 0K$ when available; see Table S4 for a discussion of experimental gaps) are listed on the top x-axes. (a) Results for Bi to AlAs (experimental band gaps 0.014 – 2.23 eV). (b) Results for GaP to BN (experimental gaps 2.35 – 6.36 eV). (c) Results for MgO to LiF (experimental gaps 7.83 – 14.2 eV)

3 Comparison of B3PW and G_0W_0 @ LDA

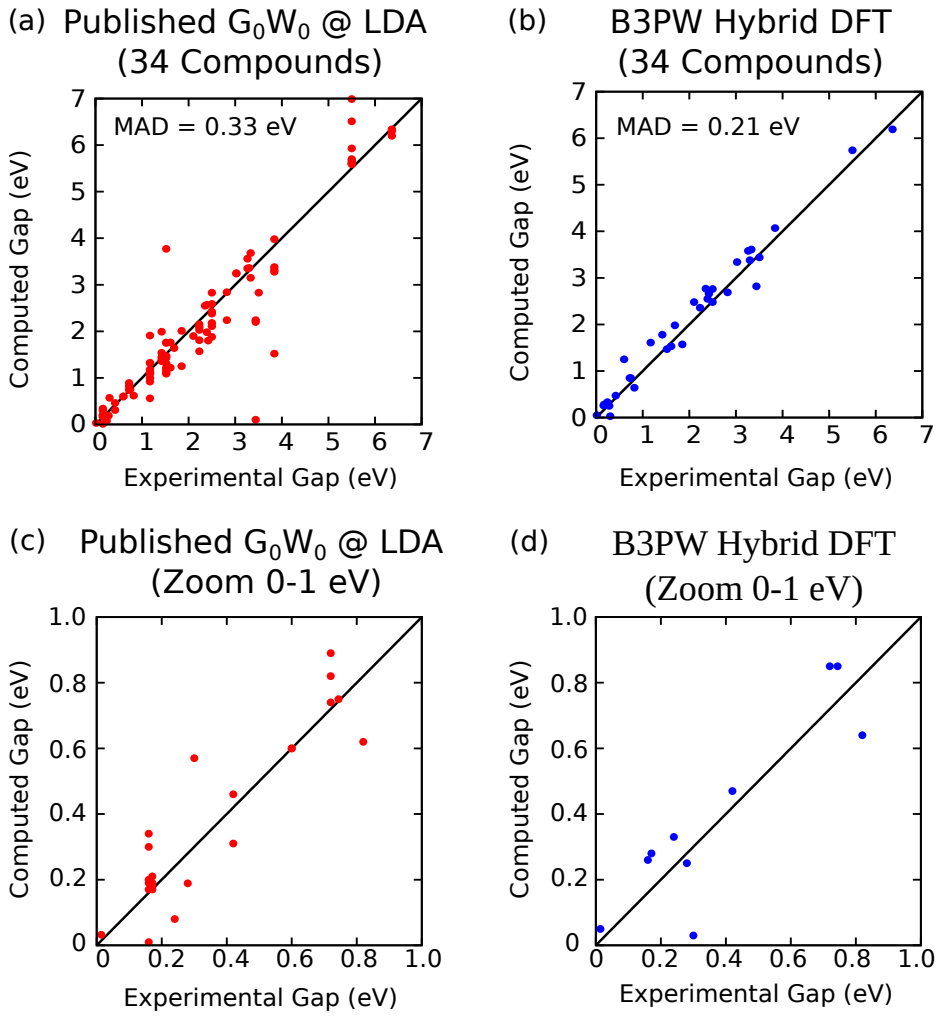

Figure S3: G_0W_0 @ LDA (G_0W_0 using LDA DFT as the starting point) and B3PW calculated band gaps versus experiment (low-temperature) for 34 compounds with band gaps below 7 eV. These 34 compounds are those for which our literature search found G_0W_0 @ LDA results, and are a subset of the 70 compounds listed in Figures 2 and 3. These 34 compounds are listed in Figure S4 (a) Published G_0W_0 @ LDA results (100 data points, 34 compounds, 22 publications). The mean absolute deviation (MAD) is 0.33 eV. (b) B3PW hybrid DFT calculations on the same 34 compounds. The MAD is 0.21 eV. (c) Zoom of (a) from 0–1 eV. (d) Zoom of (b) from 0–1 eV.

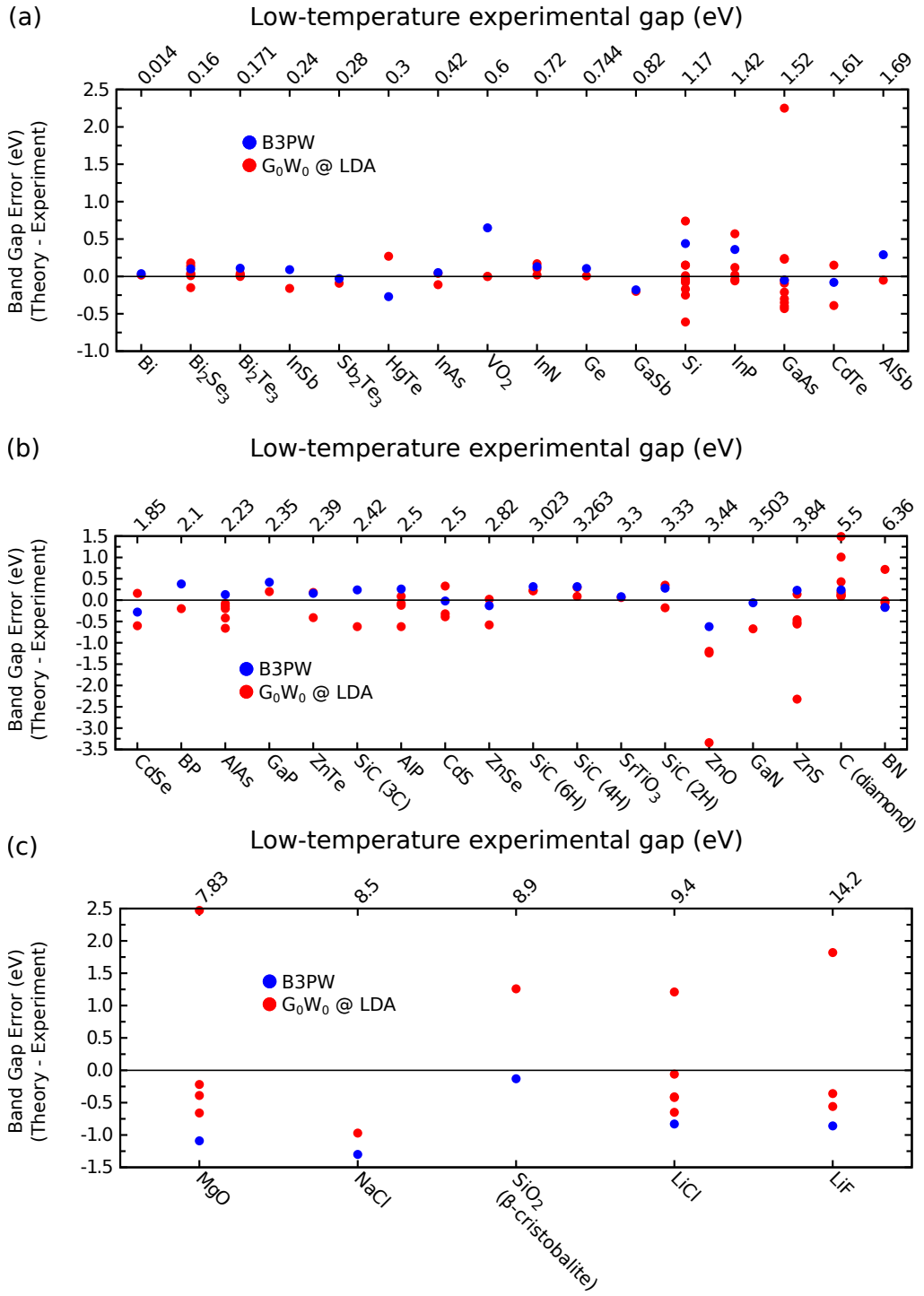

Figure S4: Difference between computed and low-temperature experimental band gaps for the 39 compounds for which our literature search found G_0W_0 @ LDA results. Our B3PW results are shown by blue circles, and red circles represent literature G_0W_0 @ LDA results. Compound names are listed on the bottom x-axes; experimental band gaps (low temperature or $T \approx 0K$ when available; see Table S4 for a discussion of experimental gaps) are listed on the top x-axes. (a) Results for Bi to AlSb (experimental band gaps 0.014 – 1.69 eV). (b) Results for CdSe to BN (experimental gaps 1.86 – 6.36 eV). (c) Results for MgO to LiF (experimental gaps 7.83 – 14.2 eV)

4 Comparison of B3PW and G_0W_0 @ PBE

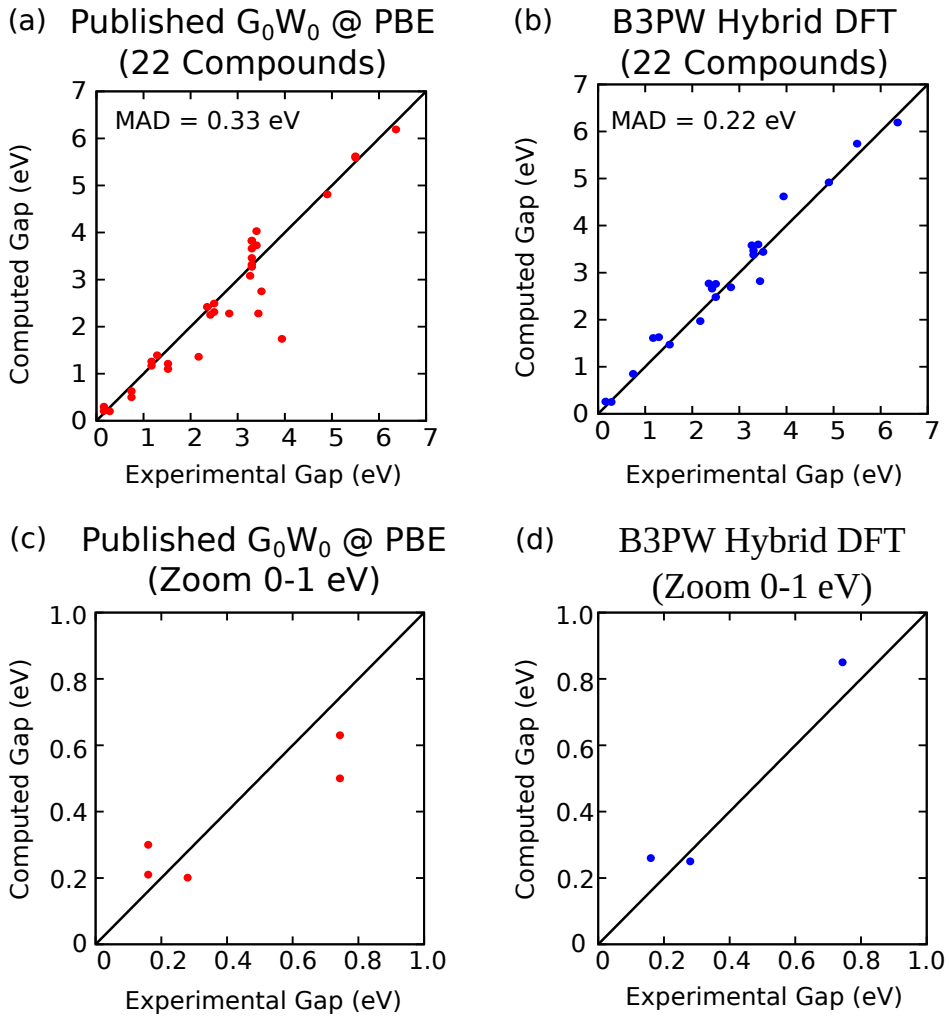

Figure S5: G_0W_0 @ PBE (G_0W_0 using PBE DFT as the starting point) and B3PW calculated band gaps versus experiment (low-temperature) for 22 compounds with gaps below 7 eV. These 22 compounds are those for which our literature search found G_0W_0 @ PBE results, and are a subset of the 70 compounds listed in Figures 2 and 3. These 22 compounds are listed in Figure S6. (a) Published G_0W_0 @ PBE results (33 data points, 22 compounds, 8 publications). The mean absolute deviation (MAD) is 0.33 eV. (b) B3PW hybrid DFT calculations on the same 22 compounds. The MAD is 0.22 eV. (c) Zoom of (a) from 0–1 eV. (d) Zoom of (b) from 0–1 eV.

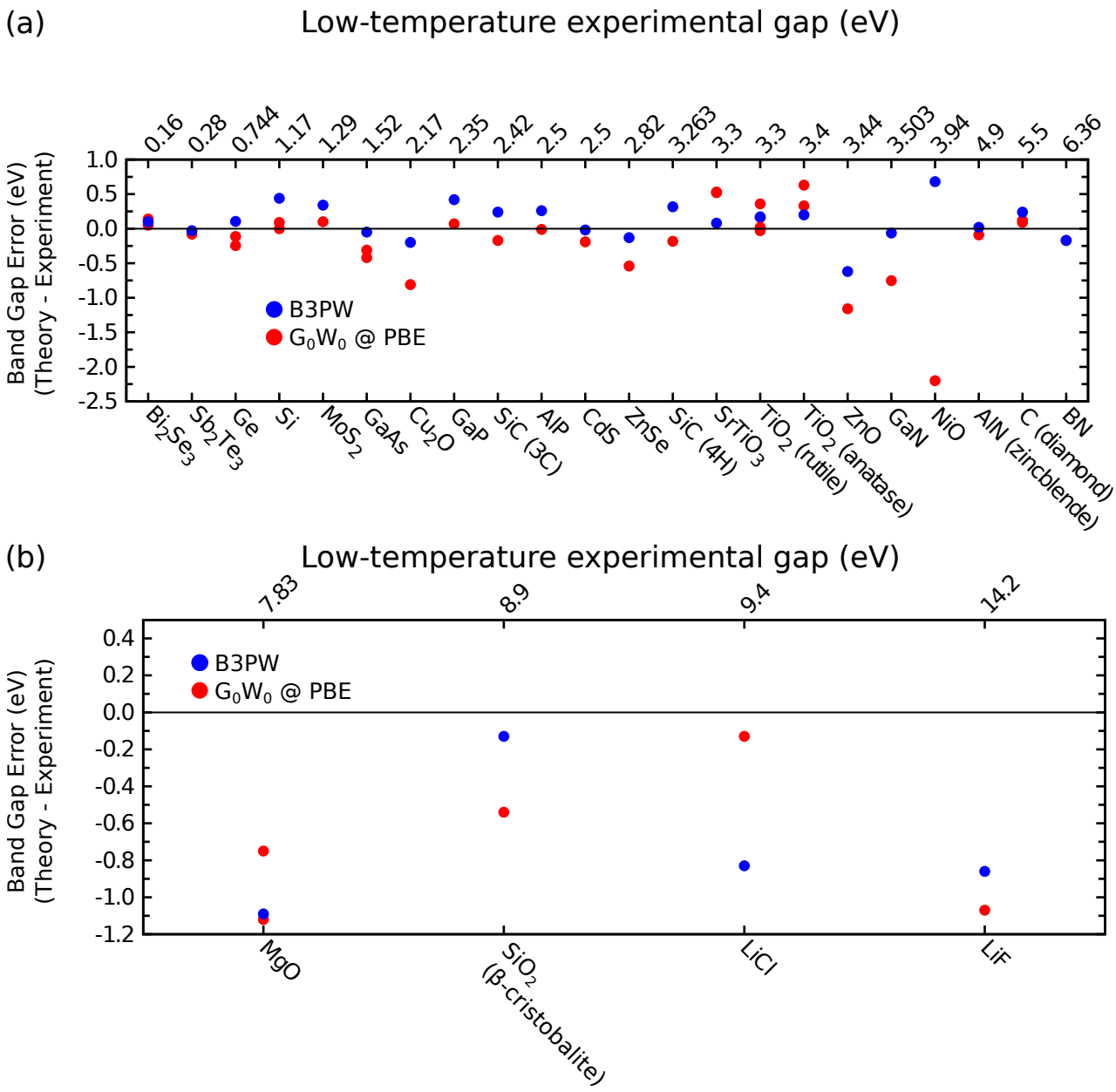

Figure S6: Difference between computed and low-temperature experimental band gaps for the 26 compounds for which our literature search found G_0W_0 @ PBE results. Our B3PW results are shown by blue circles, and red circles represent literature G_0W_0 @ PBE results. Compound names are listed on the bottom x-axes; experimental band gaps (low temperature or $T \approx 0K$ when available; see Table S4 for a discussion of experimental gaps) are listed on the top x-axes. (a) Results for Bi_2Se_3 to BN (experimental band gaps 0.16 – 6.36 eV). (b) Results for MgO to LiF (experimental gaps 7.83 – 14.2 eV)

5 Comparison of B3PW and post-G_0W_0

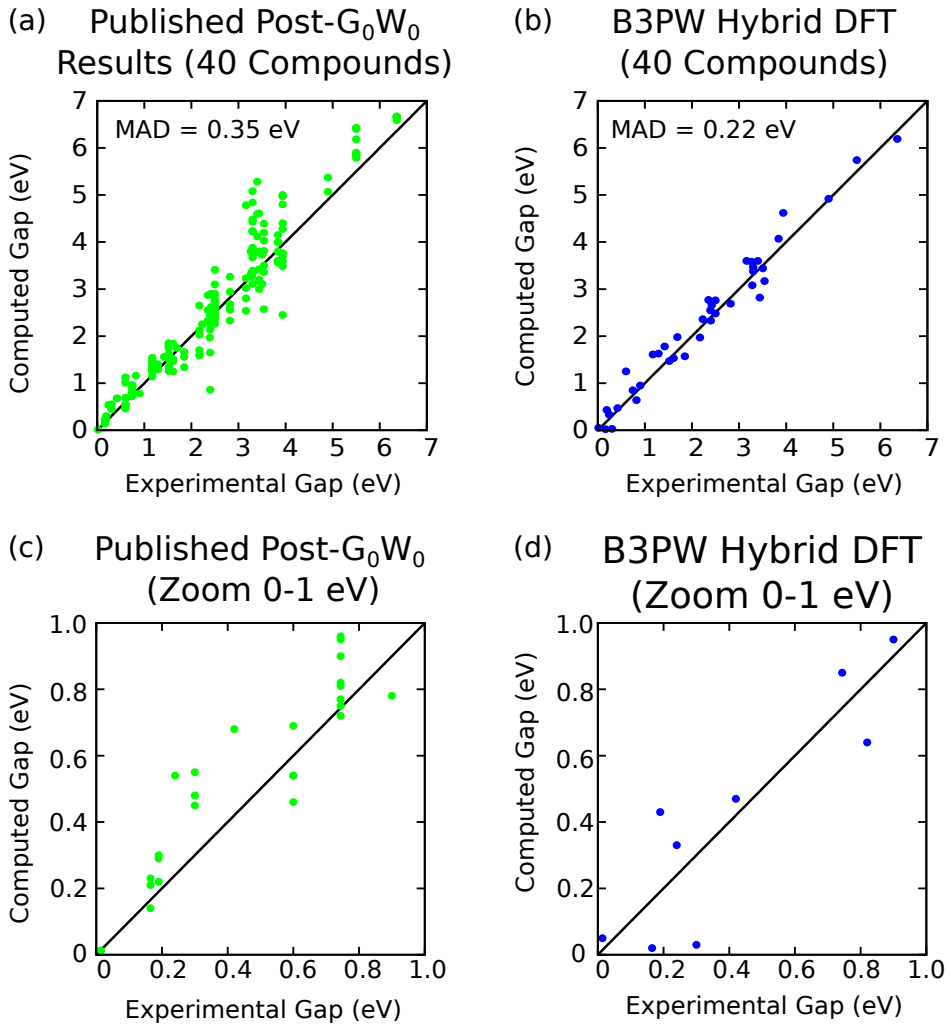

Figure S7: Post-G_0W_0 and B3PW calculated band gaps versus experiment (low-temperature) for 40 compounds with band gaps below 7 eV. These 40 compounds are those for which our literature search found post-G_0W_0 results, and are a subset of the 70 compounds listed in Figures 2 and 3. These 40 compounds are listed in Figure S8. (a) Published post-G_0W_0 results (180 data points, 40 compounds, 17 publications). The mean absolute deviation (MAD) is 0.35 eV. (b) B3PW hybrid DFT calculations on the same 40 compounds. The MAD is 0.22 eV. (c) Zoom of (a) from 0–1 eV. (d) Zoom of (b) from 0–1 eV.

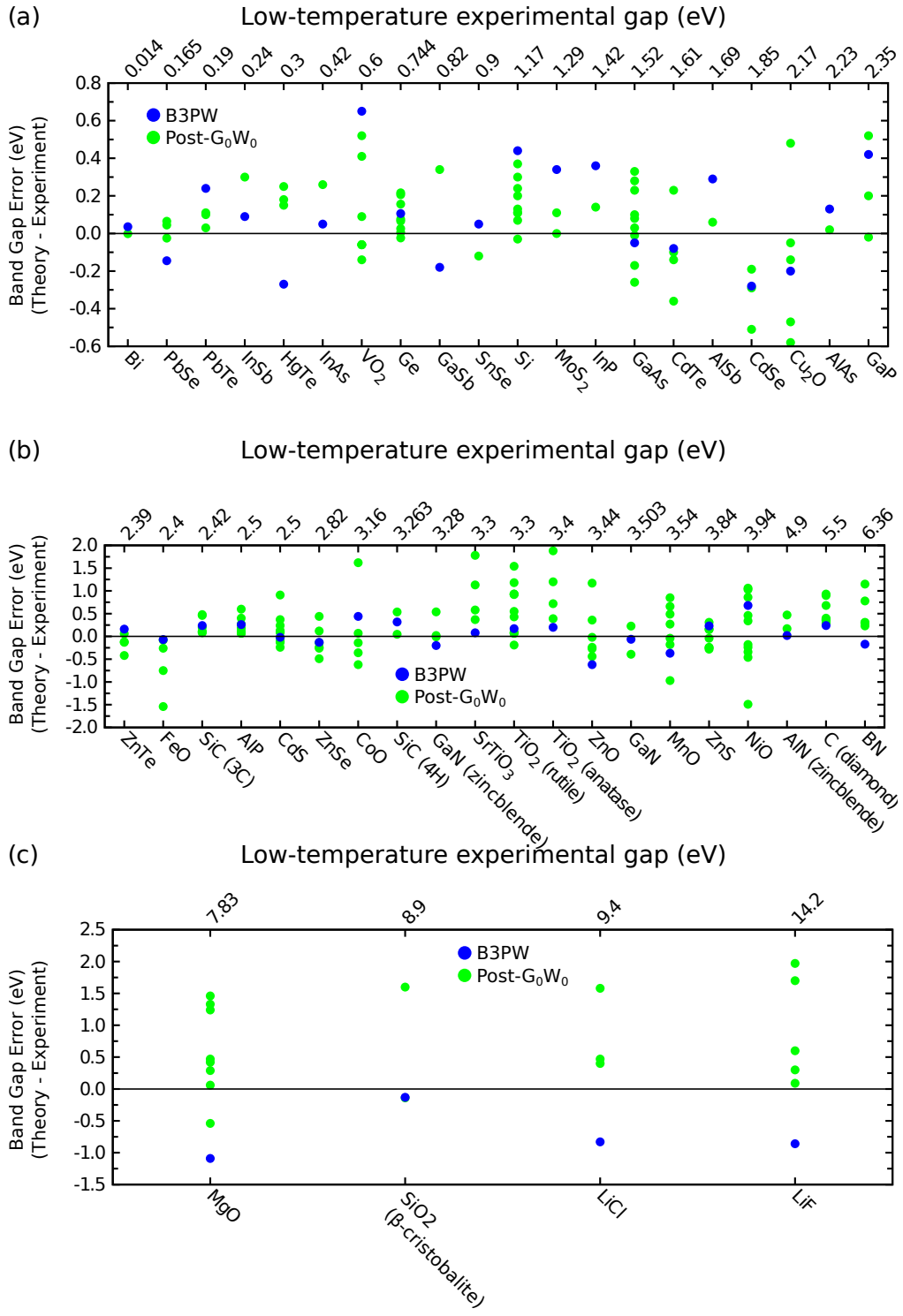

Figure S8: Difference between computed and low-temperature experimental band gaps for the 46 compounds for which our literature search found post- G_0W_0. Our B3PW results are shown by blue circles, and red circles represent literature post-G_0W_0 results. Compound names are listed on the bottom x-axes; experimental band gaps (low temperature or $T \approx 0K$ when available; see Table S4 for a discussion of experimental gaps) are listed on the top x-axes. (a) Results for Bi to GaP (experimental band gaps 0.014 – 2.35 eV). (b) Results for ZnTe to BN (experimental band gaps 2.39 – 6.36 eV). (c) Results for MgO to Ne (experimental gaps 7.83 – 21.7 eV)

6 Calculated Band Gaps Versus Low-Temperature Experiments for all Compounds

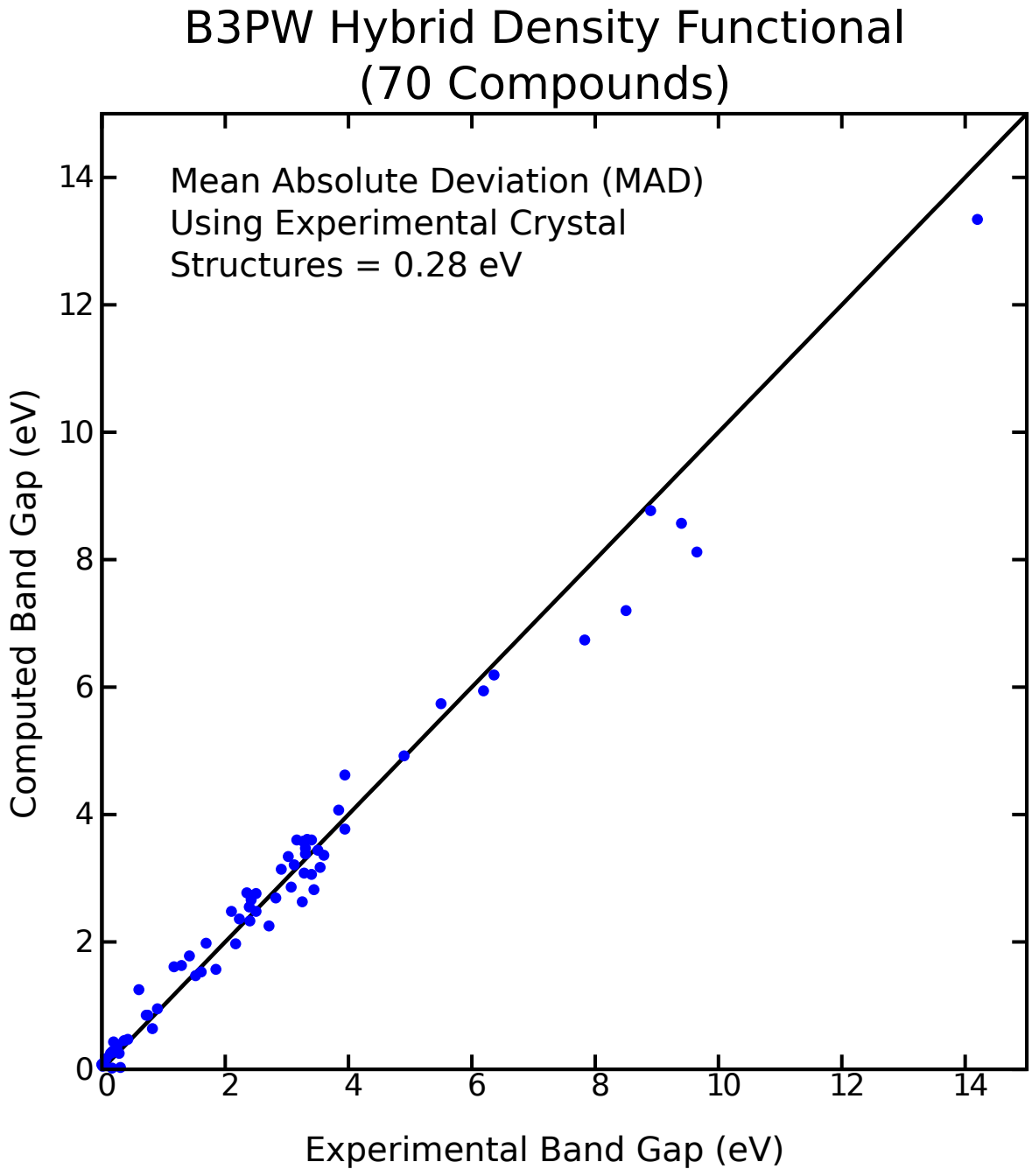

Figure S9: B3PW calculated band gaps versus experiment (low-temperature) for all 70 compounds listed in Figures 2 and 3. The mean absolute deviation is 0.28 eV.

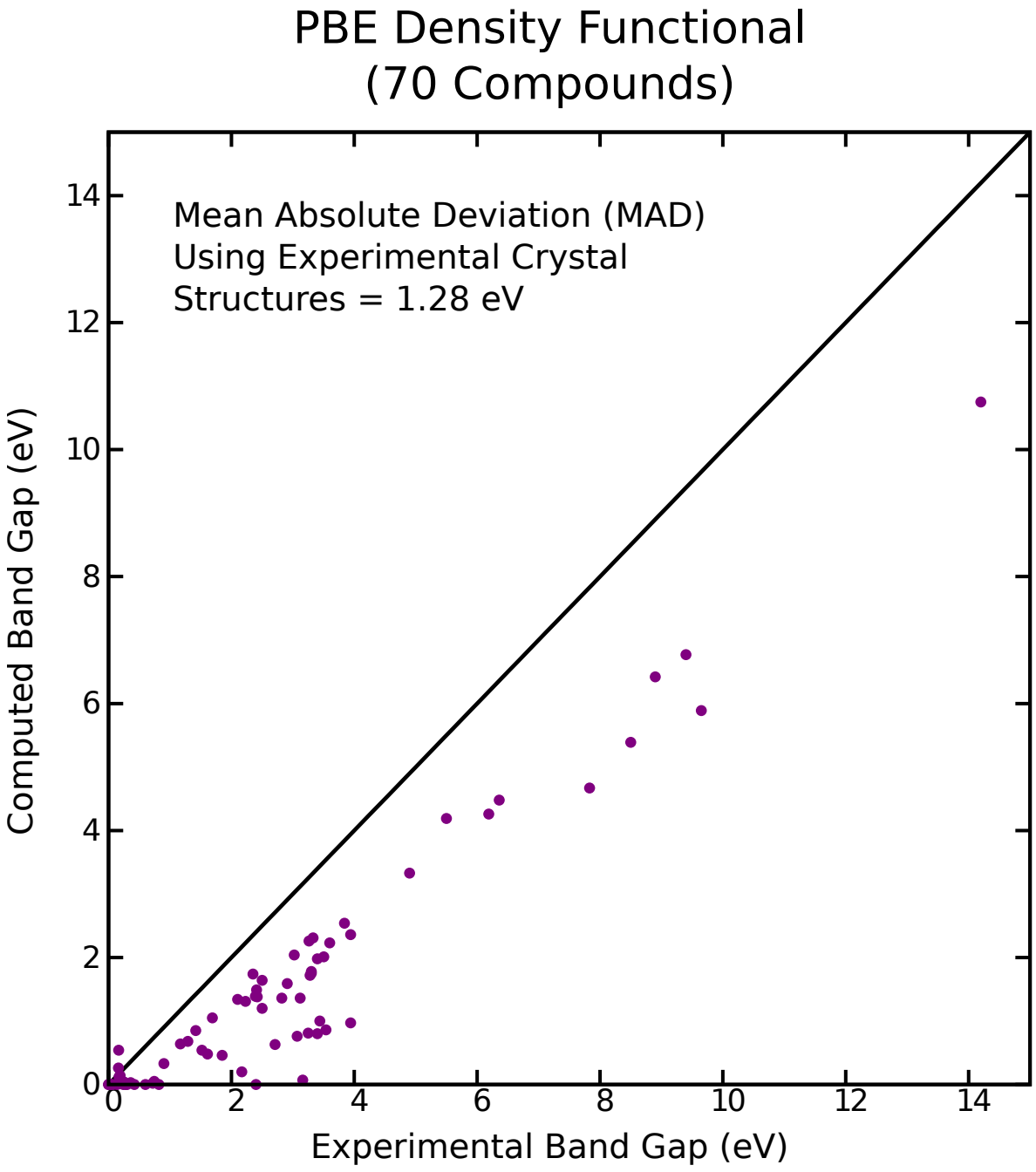

Figure S10: PBE calculated band gaps versus experiment (low-temperature) for PBE for all 70 compounds listed in Figures 2 and 3. The mean absolute deviation is 1.28 eV.

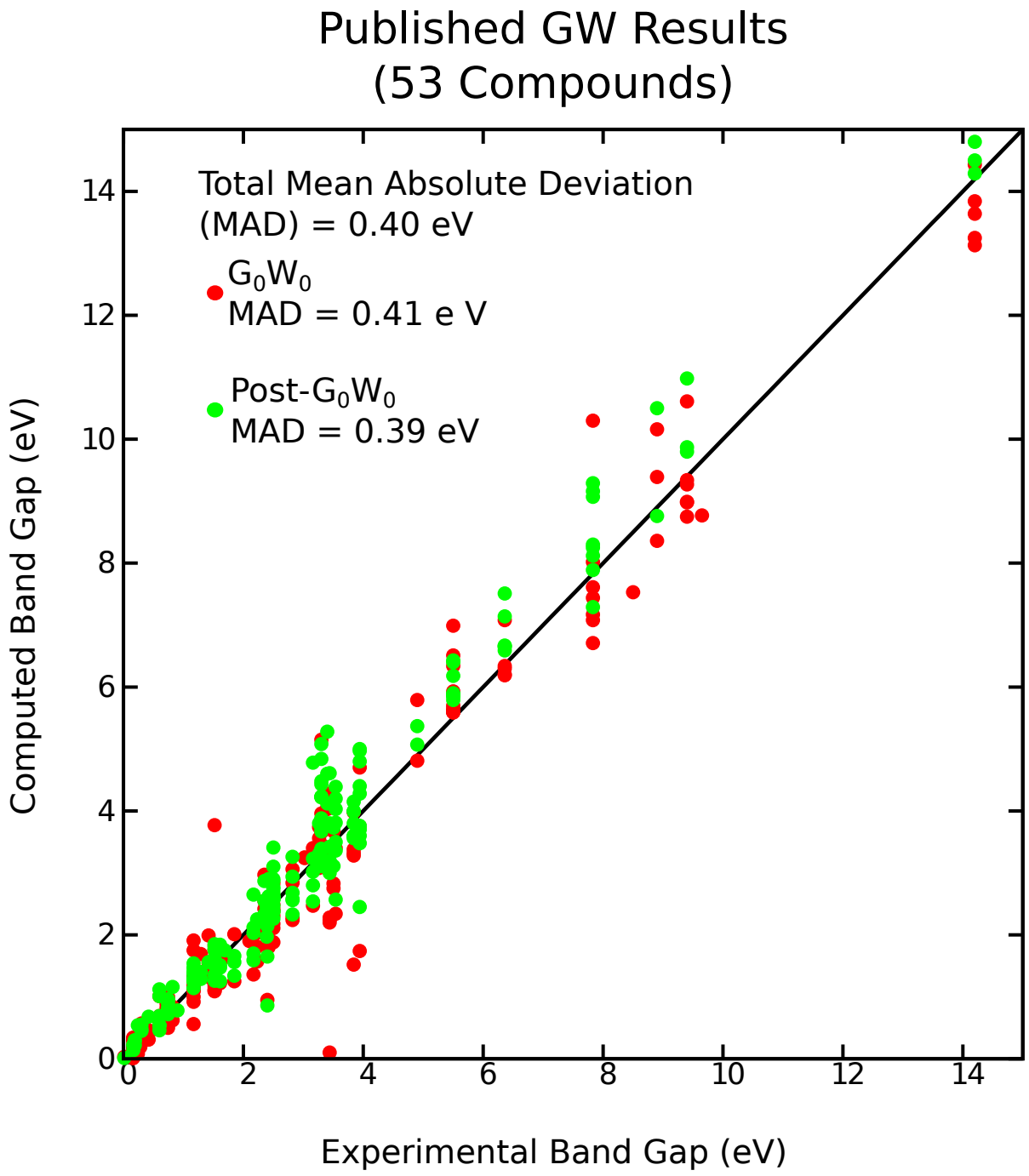

Figure S11: G_0W_0 (red circles) and post-G_0W_0 (green circles) calculated band gaps versus experiment (low-temperature) for the 53 compounds where our literature search found G_0W_0 or post-G_0W_0 results. These 53 compounds form a subset of the 70 compounds listed in Figures 2 and 3. The mean absolute deviation is 0.40 eV overall, 0.41 eV for G_0W_0, and 0.39 eV for post-G_0W_0.

7 Tables of B3PW, PBE, GW, and Experimental Band Gaps

Table S1: Band Gaps (eV) from B3PW, GW, PBE and Experiment. Red boxes link to B3PW CRYSTAL input decks. Green boxes link to references. Table S4 lists the experimental band gap from every reference.

System	B3PW	Exp	Refs	PBE	GW	Refs
Bi_2Se_3 (6 QL)	0.08	0.0	S2	0.00	N/A	N/A
Bi_2Se_3 (7 QL)	0.07	0.0	S2	0.00	N/A	N/A
Bi	0.05	0.011 – 0.015	S3–S8	0.01	0.013 – 0.032	S9
Bi_2Se_3 (5 QL)	0.12	0.04	S2	0.00	N/A	N/A
Bi_2Se_3 (4 QL)	0.17	0.07	S2	0.00	N/A	N/A
Bi_2Se_3 (3 QL)	0.25	0.14	S2	0.00	N/A	N/A
Bi_2Se_3	0.26	0.16-0.35	S3,S10	0.26	0.01–0.34	S11–S13
PbSe	0.02	0.145–0.165	S3,S14	0.54	0.14–0.23	S15,S16
Bi_2Te_3	0.28	0.13–0.171	S3,S17	0.12	0.17–0.21	S11,S13
PbTe	0.43	0.190	S14	0.14	0.22–0.3	S15,S16
InSb	0.33	0.24	S3	0.00	0.08–0.54	S18–S20
Bi_2Se_3 (2 QL)	0.39	0.25	S2	0.04	N/A	N/A
Sb_2Te_3	0.25	0.28	S3	0.00	0.189–0.201	S21
HgTe	0.03	0.3	S3	0.00	0.45–0.57	S22
SnTe	0.45	0.36	S3	0.03	N/A	N/A
InAs	0.47	0.42	S3	0.00	0.31–0.68	S18–S20,S23
VO_2	1.25	0.6	S24	0.00	0.46–1.12	S25,S26
InN	0.85	0.7 – 1.0	S27–S29	0.02	0.72 – 0.89	S30–S32
Ge	0.85	0.744	S3	0.05	0.5–1.0	S33–S36
GaSb	0.64	0.82	S3	0.00	0.62–1.16	S18–S20
SnSe	0.95	0.86–0.95	S37–S39	0.33	0.78	S40
Si	1.58	1.17	S3	0.61	0.56–1.91	S18,S23,S33–S36 S41–S44
MoS_2	1.63	1.29	S45	1.01	1.29–1.69	S35
InP	1.74	1.42	S3	0.79	1.32–1.99	S18–S20,S42,S44
GaAs	1.47	1.52	S3	0.54	1.09–3.77	S18–S20,S33–S36 S41,S42,S44,S46
CdTe	1.53	1.61	S47	0.48	1.22–1.84	S19,S22,S48
AlSb	1.98	1.69	S3	1.05	1.64–1.75	S18,S19
CdSe	1.57	1.85	S49	0.46	1.25–2.01	S22,S48
BP	2.48	2.1	S3	1.34	1.9	S50
Cu_2O	1.97	2.17	S3,S51	0.20	1.36–2.65	S26,S36
AlAs	2.36	2.23	S3	1.31	1.57–2.25	S18,S23,S42 S19,S46,S52

Table S2: Band Gaps (eV) from B3PW, GW, PBE and Experiment. Red boxes link to B3PW CRYSTAL input decks. Green boxes link to references. Table S4 lists the experimental band gap from every reference.

System	B3PW	Exp	Refs	PBE	GW	Refs
GaP	2.78	2.35	S3	1.75	2.33–2.97	S18,S19,S35
ZnTe	2.55	2.39	S3	1.39	1.97–2.67	S19,S22,S48
FeO	2.33	2.4	S53	0.00	0.86–2.32	S26,S54–S56
$BiVO_4$	2.73	2.41	S57	1.49	N/A	N/A
SiC (3C)	2.66	2.42	S3	1.38	1.8 – 2.88	S23,S34,S36
AlP	2.59	2.5	S3	1.51	1.88–3.1	S18,S34,S36 S19,S44
CdS	2.37	2.5	S49	1.12	2.11–3.41	S22,S33,S34 S36,S48,S58
AgBr	2.25	2.71	S3	0.63	N/A	N/A
ZnSe	2.69	2.82	S3	1.36	2.24–3.26	S22,S48 S19,S35
AgI	3.14	2.91	S3	1.59	N/A	N/A
SiC (6H)	3.34	3.023	S59	2.04	3.24–3.25	S60,S61
CuBr	2.86	3.07	S3	0.76	N/A	N/A
CuI	3.21	3.12	S3	1.36	N/A	N/A
CoO	3.54	2.1–5.43	S62–S66	0.13	2.4–4.78	S26,S54,S55 S56,S67,S68
AgCl	2.63	3.25	S3	0.81	N/A	N/A
SiC (4H)	3.58	3.263	S59	2.26	3.08–3.8	S35,S60,S61
GaN (zincblende)	3.08	3.28	S69	3.27 – 3.82	S34	
$SrTiO_3$	3.38	3.25–3.3	S70–S72	1.75	3.36–5.15	S33,S73,S74
TiO_2 (Rutile)	3.47	3.3	S72	1.78	3.11–4.84	S26,S74,S75 S35,S36
SiC (2H)	3.60	3.33	S76	2.30	3.15–3.68	S60,S61
CuCl	3.06	3.4	S3	0.80	N/A	N/A
TiO_2 (Anatase)	3.60	3.4	S77	1.98	3.73–5.28	S74,S75
ZnO	2.82	3.44	S3	1.00	0.1–4.61	S34,S36,S44
GaN	3.44	3.503	S3	2.01	2.75–3.82	S33–S35
MnO	3.16	2.0–4.2	S63,S78–S81	0.86	2.34–4.39	S26,S54,S55 S58,S67 S43,S56
MgTe	3.36	3.6	S82	2.23	N/A	N/A
ZnS	3.98	3.84	S49	2.46	1.52–4.15	S22,S34,S48 S19,S44
CuSCN	3.77	3.94	S83	2.36	N/A	N/A
NiO	4.57	3.7–4.3	S63,S65,S84 S66,S85	0.97	1.74–5.0	S26,S54,S55 S36,S58,S67 S43,S56

Table S3: Band Gaps (eV) from B3PW, GW, PBE and Experiment. Red boxes link to B3PW CRYSTAL input decks. Green boxes link to references. Table S4 lists the experimental band gap from every reference.

System	B3PW	Exp	Refs	PBE	GW	Refs
AlN (zincblende)	4.94	4.9	S86	3.33	N/A	N/A
C (diamond)	5.74	5.5	S3	4.19	5.59–6.99	S33,S41,S42 S35,S36 S34,S44
AlN (wurtzite)	6.05	6.19	S3	4.31	4.81–5.79	S35
BN	6.19	6.36	S87	4.48	6.19–7.51	S33,S34,S36,S44
MgO	6.79	7.83	S88	4.69	6.71–10.3	S33–S36,S44
NaCl	9.08	8.5–8.69	S89,S90	7.27	7.53	S33
SiO_2 (β-cristobalite)	8.90	8.9	S91	6.52	8.36–10.5	S35,S92
LiCl	8.76	9.4	S93	7.00	8.75–10.98	S18,S36,S41,S42
SiO_2 (α-quartz)	10.18	9.65	S94	7.79	8.77	S95
LiF	13.33	14.2	S96	10.75	13.13–16.17	S34,S35,S44,S95

8 Table of Published Experimental Band Gaps

Table S4: Experimental Band Gaps (caption on page S20). When there is more than one experimental result, our choice is in bold.

System	Band Gap (eV)	Temperature (K)	Reference
Bi_2Se_3 (6QL)	0.00	?	S2
Bi_2Se_3 (7QL)	0.00	?	S2
Bi	0.015	1.2	S7
Bi	0.015	4	S4
Bi	0.011	4	S5
Bi	0.0136	0 (extrapolated)	S6
Bi	0.0153	1.4	S8
Bi	**0.0136**	?	**S3**
Bi_2Se_3 (5QL)	0.04	?	S2
Bi_2Se_3 (4QL)	0.07	?	S2
Bi_2Se_3 (3QL)	0.14	?	S2
Bi_2Se_3	0.35	RT	S10
Bi_2Se_3	**0.16**	**77**	**S3**
PbSe	0.145	4	S3
PbSe	**0.165**	**4.2**	**S14**
Bi_2Te_3	0.13	293	S3
Bi_2Te_3	**0.171**	**0 (extrapolated)**	**S17**
PbTe	0.190	4.2	S14
InSb	0.24	1.7	S3
Bi_2Se_3 (2QL)	0.25	?	S2
Sb_2Te_3	0.28	299	S3
HgTe	0.304	0 (extrapolated)	S3
SnTe	0.36	12	S3
InAs	0.42	4.2	S3
VO_2	0.6	300	S24
InN	0.7 – 0.8	12 – 300	S27
InN	0.7 – 1.0	RT	S28
InN	**0.72**	**4–6**	**S29**
Ge	0.744	1.5	S3
GaSb	0.82	0 (extrapolated)	S3
SnSe	0.86	RT	S39
SnSe	0.898	RT	S37
SnSe	0.95	RT	S38
SnSe (average)	**0.90**		
Si	1.17	0 (extrapolated)	S3
MoS_2	1.29	?	S45
InP	1.42	1.6	S3

System	Band Gap (eV)	Temperature (K)	Reference
GaAs	1.52	0 (extrapolated)	S3
CdTe	1.48	300	S3
CdTe	**1.61**	**4.2**	**S47**
AlSb	1.69	27	S3
CdSe	1.73	300	S3
CdSe	**1.85**	**0**	**S49**
BP	2.1	RT	S3
Cu_2O	2.17	4.2	S51
Cu_2O	2.17	4.2	S3
AlAs	2.23	4	S3
GaP	2.35	0 (extrapolated)	S3
ZnTe	2.39	< 2	S3
FeO	2.4	77	S53
$BiVO_4$	2.41	?	S57
SiC (3C)	2.42	2K	S3
AlP	2.5	2	S3
CdS	2.5	300	S49
AgBr	2.71	1.8	S3
ZnSe	2.82	6	S3
AgI	2.91	4	S3
SiC (6H)	3.023	4.2	S59
CuBr	3.07	1.6	S3
CuI	3.12	80	S3
CoO	3.6	?	S62
CoO	2.6	?	S63
CoO	2.5	?	S64
CoO	2.1	78	S65
CoO	2.7	?	S66
CoO	5.43	?	S68
CoO (average)	**3.16**		
AgCl	3.25	1.8	S3
SiC (4H)	3.263	4.2	S59
GaN (zincblende)	3.28	0	S69
$SrTiO_3$	3.3	?	S72
$SrTiO_3$	3.25	?	S71
$SrTiO_3$	**3.3**	**20**	**S70**
TiO_2 (rutile)	3.3	?	S72
SiC (2H)	3.33	4.2	S76
CuCl	3.4	2	S3
TiO_2 (anatase)	3.4	0 (extrapolated)	S77
ZnO	3.44	6	S3
GaN	3.503	1.6	S3

System	Band Gap (eV)	Temperature (K)	Reference
MnO	3.6–3.8	?	S78
MnO	3.8–4.2	?	S79
MnO	4.1	?	S63
MnO	3.9	?	S80
MnO	2.0	77	S81
MnO (average)	**3.54**		
MgTe	3.49	RT	S3
MgTe	**3.6**	**0 (extrapolated)**	**S82**
ZnS	3.72	300	S3
ZnS	**3.84**	**0**	**S49**
CuSCN	3.94	RT	S83
NiO	4.3	?	S84
NiO	4.0	?	S63
NiO	4.0	78	S65
NiO	3.7	?	S85
NiO	3.7	?	S66
NiO (average)	3.94		
AlN (zincblende)	4.9	0	S86
C (diamond)	5.5	RT	S3
AlN (wurtzite)	6.19	7	S3
BN	6.2	?	S3
BN	**6.36**	**8**	**S87**
MgO	7.22	?	S97
MgO	7.9	0 (extrapolated)	S3
MgO	**7.83**	**83**	**S88**
NaCl	8.69	77	S90
NaCl	8.75	10	S98
NaCl	**8.5**	**?**	**S89**
SiO_2 (β-cristobalite)	8.9	?	S91
LiCl	9.4	55	S93
SiO_2 (α-quartz)	9.65	?	S94
LiF	14.2	77	S96

Table S4 lists the experimental band gap in every reference we found. We also list the temperature for each result or a question mark when we were unsure. In many cases there are several experimental results to choose from. When this is the case, our choice is shown in bold in Table S4. In general, when a low-temperature result from reference S3 (a standard and well-known reference work) was available, we used it. We followed this approach in all cases except the following.

PbSe. We chose reference S14, as this result is more commonly used in the literature.

Bi_2Te_3. We chose reference S17 because it is a 0 K result, whereas the band gap in S3 is at room temperature.

SnSe. We found three recent room-temperature measurements. In order to avoid biasing our comparison, we chose to average these results.

CoO, MnO, NiO. There appears to be no clear consensus as to the band gaps of these materials. We gathered the results most commonly cited in the *GW* literature and averaged. As a result, the MADs for *GW* decreased by ~ 0.01 eV and the MADs for B3PW increased by ~ 0.01 eV.

MgO and NaCl. We chose the references commonly used in the *GW* literature. This choice biases the comparison in favor of *GW*.

BP. Lucero et al.[S99] quote a low-temperature experimental band gap of 2.4 eV. This number seems plausible given the room temperature value of 2.1 eV. However, we were unable to locate any experimental paper containing this value. Thus, we used the room temperature band gap from reference S3.

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B3PW CRYSTAL Input Decks

References to the experimental structures used are shown at the top of each input deck. All experimental structures were taken from the Inorganic Crystal Structure Database (ICSD).

Bi_2Se_3 (6ql)

```
bi2se3 – Inorg Chem (1999) 38 (9) 2131
crystal
0 0 0
166
4.1355 28.615
3
283 0.000 0.000 0.4006
234 0.000 0.000 0.0000
234 0.000 0.000 0.2109
slab
0 0 1
3
30
printout
basisset
end
end
283 8
input
5. 0 2 4 2 2 0
1.994153 35.755622 0
0.240286 -0.404113 0
0.896039 2.688441 0
0.875463 5.715603 0
0.262580 -0.171255 0
0.232846 -0.150845 0
0.779775 4.060445 0
0.739216 5.980282 0
0.987519 -2.646547 0
0.959907 -3.373825 0
0 0 3 2 1
1.696224 0.519113
1.248042 -0.912045
0.365482 -0.259603
0 0 1 0 1
0.270727 1.0
0 0 1 0 1
```

0.120284 1.0
0 2 3 3 1
3.671058 0.010198
0.555533 -0.317612
0.411224 0.38604
0 2 1 0 1
0.165982 1.0
0 2 1 0 1
0.077856 1.0
0 3 1 0 1
0.256 1.0
0 3 1 0 1
0.134 1.0
234 9
input
24. 0 2 4 6 2
30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280

1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1
0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1
100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
sorestart
tolinteg
9 7 7 7 14

```
end
10 0 20
maxcycle
1
fmixing
80
broyden
0.01
ppan
end
```

Bi_2Se_3 (7QL)

bi2se3 – Inorg Chem (1999) 38 (9) 2131
crystal
0 0 0
166
4.1355 28.615
3
283 0.000 0.000 0.4006
234 0.000 0.000 0.0000
234 0.000 0.000 0.2109
slab
0 0 1
3
35
printout
basisset
end
end
283 8
input
5. 0 2 4 2 2 0
1.994153 35.755622 0
0.240286 -0.404113 0
0.896039 2.688441 0
0.875463 5.715603 0
0.262580 -0.171255 0
0.232846 -0.150845 0
0.779775 4.060445 0
0.739216 5.980282 0
0.987519 -2.646547 0
0.959907 -3.373825 0
0 0 3 2 1
1.696224 0.519113
1.248042 -0.912045
0.365482 -0.259603
0 0 1 0 1
0.270727 1.0
0 0 1 0 1
0.120284 1.0
0 2 3 3 1
3.671058 0.010198
0.555533 -0.317612
0.411224 0.38604
0 2 1 0 1

0.165982 1.0
0 2 1 0 1
0.077856 1.0
0 3 1 0 1
0.256 1.0
0 3 1 0 1
0.134 1.0
234 9
input
24. 0 2 4 6 2
30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1

0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1
100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
9 7 7 7 14
end
10 0 20
maxcycle
20
fmixing
80
broyden

0.01
ppan
end

Bi

bi – Acta Crystallographica 1962 15 865
crystal
0 0 0
166
4.546 11.862
1
283 0.000 0.000 0.2339
end
283 9
input
23. 0 2 4 4 2
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10.467777 72.001499 0
9.118901 144.002277 0
6.754791 5.007945 0
6.252592 9.991550 0
8.081474 36.396259 0
7.890595 54.597664 0
4.955556 9.984294 0
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4.133400 18.194308 0
0 0 8 2 1
211.821 0.001088
21.3262 -0.105862
13.3654 0.530808
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1.71229 0.995856
0.839107 0.398952
0.255364 0.011778
0.096700 -0.001470
0 0 8 2 1
211.821 0.000422
21.3262 -0.038537
13.3654 0.217238
6.94610 -0.481097
1.71229 0.701595
0.839107 0.290520
0.255364 -0.799778
0.096700 -0.496131
0 0 1 0 1
0.255364 1

0 0 1 0 1
0.096700 1
0 2 6 6 1
11.0644 0.167249
7.45000 -0.425262
2.01069 0.692525
0.888321 0.475374
0.236369 0.029859
0.079290 -0.004493
0 2 6 3 1
11.0644 -0.052201
7.45000 0.139083
2.01069 -0.293556
0.888321 -0.158574
0.236369 0.574362
0.079290 0.572678
0 2 1 0 1
0.079290 1
0 3 6 10 1
16.2461 0.007808
6.98363 -0.066831
2.37476 0.324140
1.15372 0.485831
0.525974 0.301056
0.2151 0.063196
0 3 1 0 1
0.2151 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
9 7 7 7 14
tolpseud
7
end
12 0 24
maxcycle
100
fmixing
80

broyden
0.0001
tolscf
8 8
ppan
end

Bi_2Se_3 (5QL)

bi2se3 – Inorg Chem (1999) 38 (9) 2131
crystal
0 0 0
166
4.1355 28.615
3
283 0.000 0.000 0.4006
234 0.000 0.000 0.0000
234 0.000 0.000 0.2109
slab
0 0 1
3
25
printout
basisset
end
end
283 8
input
5. 0 2 4 2 2 0
1.994153 35.755622 0
0.240286 -0.404113 0
0.896039 2.688441 0
0.875463 5.715603 0
0.262580 -0.171255 0
0.232846 -0.150845 0
0.779775 4.060445 0
0.739216 5.980282 0
0.987519 -2.646547 0
0.959907 -3.373825 0
0 0 3 2 1
1.696224 0.519113
1.248042 -0.912045
0.365482 -0.259603
0 0 1 0 1
0.270727 1.0
0 0 1 0 1
0.120284 1.0
0 2 3 3 1
3.671058 0.010198
0.555533 -0.317612
0.411224 0.38604
0 2 1 0 1

0.165982 1.0
0 2 1 0 1
0.077856 1.0
0 3 1 0 1
0.256 1.0
0 3 1 0 1
0.134 1.0
234 9
input
24. 0 2 4 6 2
30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1

0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1
100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
9 7 7 7 14
end
10 0 20
maxcycle
20
fmixing
80
broyden

0.01
ppan
end

Bi_2Se_3 (4QL)

bi2se3 – Inorg Chem (1999) 38 (9) 2131
crystal
0 0 0
166
4.1355 28.615
3
283 0.000 0.000 0.4006
234 0.000 0.000 0.0000
234 0.000 0.000 0.2109
slab
0 0 1
3
20
printout
basisset
end
end
283 8
input
5. 0 2 4 2 2 0
1.994153 35.755622 0
0.240286 -0.404113 0
0.896039 2.688441 0
0.875463 5.715603 0
0.262580 -0.171255 0
0.232846 -0.150845 0
0.779775 4.060445 0
0.739216 5.980282 0
0.987519 -2.646547 0
0.959907 -3.373825 0
0 0 3 2 1
1.696224 0.519113
1.248042 -0.912045
0.365482 -0.259603
0 0 1 0 1
0.270727 1.0
0 0 1 0 1
0.120284 1.0
0 2 3 3 1
3.671058 0.010198
0.555533 -0.317612
0.411224 0.38604
0 2 1 0 1

0.165982 1.0
0 2 1 0 1
0.077856 1.0
0 3 1 0 1
0.256 1.0
0 3 1 0 1
0.134 1.0
234 9
input
24. 0 2 4 6 2
30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1

0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1
100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
9 7 7 7 14
end
10 0 20
maxcycle
20
fmixing
80
broyden

0.01
ppan
end

Bi_2Se_3 (3QL)

bi2se3 – Inorg Chem (1999) 38 (9) 2131
crystal
0 0 0
166
4.1355 28.615
3
283 0.000 0.000 0.4006
234 0.000 0.000 0.0000
234 0.000 0.000 0.2109
slab
0 0 1
3
15
printout
basisset
end
end
283 8
input
5. 0 2 4 2 2 0
1.994153 35.755622 0
0.240286 -0.404113 0
0.896039 2.688441 0
0.875463 5.715603 0
0.262580 -0.171255 0
0.232846 -0.150845 0
0.779775 4.060445 0
0.739216 5.980282 0
0.987519 -2.646547 0
0.959907 -3.373825 0
0 0 3 2 1
1.696224 0.519113
1.248042 -0.912045
0.365482 -0.259603
0 0 1 0 1
0.270727 1.0
0 0 1 0 1
0.120284 1.0
0 2 3 3 1
3.671058 0.010198
0.555533 -0.317612
0.411224 0.38604
0 2 1 0 1

0.165982 1.0
0 2 1 0 1
0.077856 1.0
0 3 1 0 1
0.256 1.0
0 3 1 0 1
0.134 1.0
234 9
input
24. 0 2 4 6 2
30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1

0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1
100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
9 7 7 7 14
end
10 0 20
maxcycle
20
fmixing
80
broyden

0.01
ppan
end

Bi_2Se_3

bi2se3 – Inorg Chem (1999) 38 (9) 2131
crystal
0 0 0
166
4.1355 28.615
3
283 0.000 0.000 0.4006
234 0.000 0.000 0.0000
234 0.000 0.000 0.2109
end
283 8
input
5. 0 2 4 2 2 0
1.994153 35.755622 0
0.240286 -0.404113 0
0.896039 2.688441 0
0.875463 5.715603 0
0.262580 -0.171255 0
0.232846 -0.150845 0
0.779775 4.060445 0
0.739216 5.980282 0
0.987519 -2.646547 0
0.959907 -3.373825 0
0 0 3 2 1
1.696224 0.519113
1.248042 -0.912045
0.365482 -0.259603
0 0 1 0 1
0.270727 1.0
0 0 1 0 1
0.120284 1.0
0 2 3 3 1
3.671058 0.010198
0.555533 -0.317612
0.411224 0.38604
0 2 1 0 1
0.165982 1.0
0 2 1 0 1
0.077856 1.0
0 3 1 0 1
0.256 1.0
0 3 1 0 1
0.134 1.0

234 9
input
24. 0 2 4 6 2
30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1
0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283

0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1
100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
9 7 7 7 14
end
10 0 20
maxcycle
20
fmixing
80
broyden
0.01
end

PbSe

PbSe – Acta Crystallographica, Section B: Structural Science (1983) 39, p312-p317
crystal
0 0 0
225
6.128
2
282 0.5 0.5 0.5
234 0.00 0.00 0.00
printout
basisset
end
end
282 8
input
4. 0 2 4 2 2 0
1.940106 35.775442 0
0.275063 -0.558568 0
0.921930 2.609796 0
0.903965 5.553646 0
0.256555 -0.151563 0
0.189112 -0.090292 0
0.664793 2.956364 0
0.621886 4.242489 0
0.813760 -2.144958 0
0.779307 -2.666379 0
0 0 3 2 1
1.576075 0.499998
1.157411 -0.874119
0.340937 -0.298476
0 0 1 0 1
0.252448 1.0
0 0 1 0 1
0.109434 1.0
0 2 3 2 0 1
2.836533 0.007303
0.604749 -0.206213
0.442006 0.173019
0 2 1 0 1
0.180638 1.0
0 2 1 0 1
0.082396 1.0
0 3 1 0 1
0.2306 1.0

0 3 1 0 1
0.1142 1.0
234 9
input
24. 0 2 4 6 2
30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1
0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655

2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1
100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 9 30
end
12 0 24
maxcycle
100
fmixing
80
broyden
0.0001
tolscf
7 7
end

Bi_2Te_3

bi2te3– Materials Research Bulletin (1993) 28, p591-p596
crystal
0 0 0
166
4.395 30.440
3
283 0.000 0.000 0.4005
252 0.000 0.000 0.0000
252 0.000 0.000 0.2097
printout
basisset
end
end
283 8
input
5. 0 2 4 2 2 0
1.994153 35.755622 0
0.240286 -0.404113 0
0.896039 2.688441 0
0.875463 5.715603 0
0.262580 -0.171255 0
0.232846 -0.150845 0
0.779775 4.060445 0
0.739216 5.980282 0
0.987519 -2.646547 0
0.959907 -3.373825 0
0 0 3 2 1
1.696224 0.519113
1.248042 -0.912045
0.365482 -0.259603
0 0 1 0 1
0.270727 1.0
0 0 1 0 1
0.120284 1.0
0 2 3 3 1
3.671058 0.010198
0.555533 -0.317612
0.411224 0.38604
0 2 1 0 1
0.165982 1.0
0 2 1 0 1
0.077856 1.0
0 3 1 0 1

0.256 1.0
0 3 1 0 1
0.134 1.0
252 6
input
6. 0 2 4 2 2 0
2.656483 50.217674 0
2.281974 1.982941 0
2.946988 39.938015 0
2.790001 79.873384 0
1.750168 -0.651126 0
1.909579 -1.288332 0
1.107233 5.059096 0
1.084059 7.498701 0
1.992613 -7.997183 0
1.968281 -10.464938 0
0 0 3 2 1
4.620870 -0.076259
3.407086 0.222163
1.353795 -0.541514
0 0 1 0 1
0.278218 1.0
0 0 1 0 1
0.128403 1.0
0 2 3 4 1
4.772823 -0.038412
3.508559 0.112992
1.653984 -0.229605
0 2 1 0 1
0.326880 1.0
0 2 1 0 1
0.139746 1.0
99 0
end
uhf
dft
b3pw
end
biesplit
10
sorestart
end
10 0 20
maxcycle
100

fmixing
60
broyden
0.01
ppan
end

PbTe

PbTe – Acta Crystallographica, Section B: Structural Science (1983) 39, p312-p317
crystal
0 0 0
225
6.462
2
282 0.5 0.5 0.5
252 0.00 0.00 0.00
printout
basisset
end
end
282 8
input
4. 0 2 4 2 2 0
1.940106 35.775442 0
0.275063 -0.558568 0
0.921930 2.609796 0
0.903965 5.553646 0
0.256555 -0.151563 0
0.189112 -0.090292 0
0.664793 2.956364 0
0.621886 4.242489 0
0.813760 -2.144958 0
0.779307 -2.666379 0
0 0 3 2 1
1.576075 0.499998
1.157411 -0.874119
0.340937 -0.298476
0 0 1 0 1
0.252448 1.0
0 0 1 0 1
0.109434 1.0
0 2 3 2 0 1
2.836533 0.007303
0.604749 -0.206213
0.442006 0.173019
0 2 1 0 1
0.180638 1.0
0 2 1 0 1
0.082396 1.0
0 3 1 0 1
0.2306 1.0

0 3 1 0 1
0.1142 1.0
252 6
input
6. 0 2 4 2 2 0
2.656483 50.217674 0
2.281974 1.982941 0
2.946988 39.938015 0
2.790001 79.873384 0
1.750168 -0.651126 0
1.909579 -1.288332 0
1.107233 5.059096 0
1.084059 7.498701 0
1.992613 -7.997183 0
1.968281 -10.464938 0
0 0 3 2 1
4.620870 -0.076259
3.407086 0.222163
1.353795 -0.541514
0 0 1 0 1
0.278218 1.0
0 0 1 0 1
0.128403 1.0
0 2 3 4 1
4.772823 -0.038412
3.508559 0.112992
1.653984 -0.229605
0 2 1 0 1
0.326880 1.0
0 2 1 0 1
0.139746 1.0
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 9 30
end
12 0 24
maxcycle
100

fmixing
80
broyden
0.0001
tolscf
7 7
end

InSb

InSb – Materials Chemistry and Physics (2008) 112, p745-p748
crystal
0 0 0
216
6.476
2
249 0. 0. 0.
251 0.25 0.25 0.25
printout
basisset
end
end
249 9
input
21. 0 2 4 4 2
15.392822 281.122350 0
8.055864 61.901470 0
13.928672 67.462154 0
13.347234 134.949250 0
7.614132 14.746140 0
7.318365 29.639262 0
14.034715 35.493254 0
14.511616 53.178773 0
5.550550 9.177281 0
5.059415 12.392410 0
12.539056 -13.728078 0
12.552561 -18.206866 0
0 0 8 2 1
265.131 0.000770
25.5694 -0.052791
16.0041 0.259343
6.81885 -0.739289
1.66676 0.885773
0.769232 0.442592
0.170415 0.011574
0.1 -0.002451
0 0 8 2 1
265.131 -0.000230
25.5694 0.014088
16.0041 -0.078615
6.81885 0.252864
1.66676 -0.415545
0.769232 -0.296647

0.170415 0.678578
0.1 0.527129
0 0 1 0 1
0.170415 1
0 0 1 0 1
0.1 1
0 2 6 6 1
14.4691 0.090177
9.28083 -0.267642
2.08201 0.664483
0.844314 0.461690
0.186900 0.027059
0.1 -0.004677
0 2 6 1 1
14.4691 -0.019023
9.28083 0.059157
2.08201 -0.180749
0.844314 -0.114582
0.186900 0.440739
0.1 0.687789
0 2 1 0 1
0.1 1
0 3 6 10 1
30.7879 0.005766
19.2555 -0.010708
3.19662 0.293860
1.33210 0.510869
0.504619 0.341519
0.1498 0.052465
0 3 1 0 1
0.1498 1
251 9
input
23. 0 2 4 4 2 0
16.330865 281.071581 0
8.556542 61.716604 0
14.470337 67.457380 0
13.816194 134.933503 0
8.424924 14.716344 0
8.092728 29.518512 0
14.886331 35.447815 0
15.146319 53.143466 0
5.908267 9.179223 0
5.594322 13.240253 0
14.444978 -15.366801 0

14.449295 -20.296138 0
0 0 8 2. 1
371.584 0.001591
26.5392 -0.041684
16.6213 0.273343
7.73551 -0.767685
1.89234 0.899496
0.910431 0.431387
0.244231 0.012837
0.092397 -0.002173
0 0 8 2. 1
371.584 0.000654
26.5392 -0.010962
16.6213 0.093833
7.73551 -0.304009
1.89234 0.508409
0.910431 0.339239
0.244231 -0.734772
0.092397 -0.526134
0 0 1 0. 1
0.244231 1
0 0 1 0. 1
0.092397 1
0 2 6 6. 1
16.0509 0.092157
10.2621 -0.275559
2.42832 0.65864
1.03360 0.466892
0.25944 0.028511
0.086108 -0.005155
0 2 6 3. 1
16.0509 -0.025313
10.2621 0.079796
2.42832 -0.242094
1.03360 -0.148605
0.25944 0.548944
0.086108 0.589291
0 2 1 0. 1
0.086108 1
0 3 6 10. 1
45.4785 0.003259
18.5114 -0.005497
3.91600 0.279953
1.71482 0.512751
0.697319 0.332872

0.2304 0.048843
0 3 1 0. 1
0.2304 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.001
end

Bi_2Se_3 (2QL)

bi2se3 – Inorg Chem (1999) 38 (9) 2131
crystal
0 0 0
166
4.1355 28.615
3
283 0.000 0.000 0.4006
234 0.000 0.000 0.0000
234 0.000 0.000 0.2109
slab
0 0 1
3
10
printout
basisset
end
end
283 8
input
5. 0 2 4 2 2 0
1.994153 35.755622 0
0.240286 -0.404113 0
0.896039 2.688441 0
0.875463 5.715603 0
0.262580 -0.171255 0
0.232846 -0.150845 0
0.779775 4.060445 0
0.739216 5.980282 0
0.987519 -2.646547 0
0.959907 -3.373825 0
0 0 3 2 1
1.696224 0.519113
1.248042 -0.912045
0.365482 -0.259603
0 0 1 0 1
0.270727 1.0
0 0 1 0 1
0.120284 1.0
0 2 3 3 1
3.671058 0.010198
0.555533 -0.317612
0.411224 0.38604
0 2 1 0 1

0.165982 1.0
0 2 1 0 1
0.077856 1.0
0 3 1 0 1
0.256 1.0
0 3 1 0 1
0.134 1.0
234 9
input
24. 0 2 4 6 2
30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1

0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1
100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
9 7 7 7 14
end
10 0 20
maxcycle
20
fmixing
80
broyden

0.01
ppan
end

Sb_2Te_3

sb2te3– Acta Crystallographica B (24,1968-38,1982) (1974) 30, p1307-p1310
crystal
0 0 0
166
4.2640 30.458
3
251 0.000 0.000 0.3988
252 0.000 0.000 0.0000
252 0.000 0.000 0.2128
printout
basisset
end
end
251 6
input
5. 0 2 4 2 2 0
2.332041 67.892881 0
1.376531 -7.420586 0
2.226128 18.864130 0
2.121810 37.723024 0
1.243157 -0.736364 0
1.316596 -1.516824 0
0.930013 3.774218 0
0.912651 5.637552 0
1.631791 -6.368730 0
1.609802 -8.315509 0
0 0 3 2 1
1.817000 0.717271
1.336276 -1.399583
0.984000 0.321171
0 0 1 0 1
0.218237 1.0
0 0 1 0 1
0.094049 1.0
0 2 3 3 1
2.061268 0.140755
1.526865 -0.276063
0.303261 0.328800
0 2 1 0 1
0.148617 1.0
0 2 1 0 1
0.074125 1.0
252 6

```
input
6.  0 2 4 2 2 0
2.656483 50.217674 0
2.281974 1.982941 0
2.946988 39.938015 0
2.790001 79.873384 0
1.750168 -0.651126 0
1.909579 -1.288332 0
1.107233 5.059096 0
1.084059 7.498701 0
1.992613 -7.997183 0
1.968281 -10.464938 0
0 0 3 2 1
4.620870 -0.076259
3.407086 0.222163
1.353795 -0.541514
0 0 1 0 1
0.278218 1.0
0 0 1 0 1
0.128403 1.0
0 2 3 4 1
4.772823 -0.038412
3.508559 0.112992
1.653984 -0.229605
0 2 1 0 1
0.326880 1.0
0 2 1 0 1
0.139746 1.0
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
10 0 20
maxcycle
50
tolscf
7 7
fmixing
```

80
broyden
0.0001
end

HgTe

HgTe – Journal of Physics and Chemistry of Solids (1960) 15, p27-p32
crystal
0 0 0
216
6.460
2
280 0.000 0.000 0.000
252 0.25 0.25 0.25
printout
basisset
end
end
280 8
input
20. 0 2 4 4 2 0
12.413071 275.774797 0
6.897913 49.267898 0
11.310320 80.506984 0
10.210773 161.034824 0
5.939804 9.083416 0
5.019755 18.367773 0
8.407895 51.137256 0
8.214086 76.707459 0
4.012612 6.561821 0
3.795398 9.818070 0
3.273106 9.429001 0
3.208321 12.494856 0
0 0 7 2 1
0.41480400E+02 0.10072000E-01
0.22532800E+02 -0.11478100E+00
0.14079000E+02 0.35640800E+00
0.57247400E+01 -0.84844300E+00
0.14794800E+01 0.94059600E+00
0.68826600E+00 0.43532900E+00
0.16418100E+00 0.13178000E-01
0 0 7 2 1
0.41480400E+02 0.20320000E-02
0.22532800E+02 -0.32314000E-01
0.14079000E+02 0.11535000E+00
0.57247400E+01 -0.31776300E+00
0.14794800E+01 0.51352300E+00
0.68826600E+00 0.25005000E+00
0.16418100E+00 -0.64884100E+00

0 0 1 0 1
0.16418100E+00 -0.10536460E+01
0 0 1 0 1
0.1 0.10000000E+01
0 2 6 6 1
0.10580500E+02 0.12869200E+00
0.68053900E+01 -0.36084200E+00
0.17901600E+01 0.56411700E+00
0.86226100E+00 0.50027400E+00
0.37527700E+00 0.11378500E+00
0.12842100E+00 0.29390000E-02
0 2 1 0 1
0.1 0.10000000E+01
0 3 6 10 1
0.11584100E+02 0.16729000E-01
0.72487900E+01 -0.69558000E-01
0.19366200E+01 0.30343700E+00
0.89874800E+00 0.45487800E+00
0.38693100E+00 0.33680800E+00
0.15046600E+00 0.11301600E+00
0 3 1 0 1
0.15046600E+00 0.10000000E+01
252 6
input
6. 0 2 4 2 2 0
2.656483 50.217674 0
2.281974 1.982941 0
2.946988 39.938015 0
2.790001 79.873384 0
1.750168 -0.651126 0
1.909579 -1.288332 0
1.107233 5.059096 0
1.084059 7.498701 0
1.992613 -7.997183 0
1.968281 -10.464938 0
0 0 3 2 1
4.620870 -0.076259
3.407086 0.222163
1.353795 -0.541514
0 0 1 0 1
0.278218 1.0
0 0 1 0 1
0.128403 1.0
0 2 3 4 1
4.772823 -0.038412

3.508559 0.112992
1.653984 -0.229605
0 2 1 0 1
0.326880 1.0
0 2 1 0 1
0.139746 1.0
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

SnTe

SnTe – Physica Status Solidi B - Basic Solid State Physics (2013) 250, (7) p1300-p1307
crystal
0 0 0
225
6.318
2
250 0.000 0.000 0.000
252 0.5 0.5 0.5
printout
basisset
end
end
250 9
input
22. 0 2 4 4 2 0
17.420414 279.988682 0
7.631155 62.377810 0
16.131024 66.162523 0
15.628077 132.174396 0
7.325608 16.339417 0
6.942519 32.488959 0
15.514976 36.387441 0
15.188160 54.507841 0
5.456024 8.696823 0
5.363105 12.840208 0
12.282348 -12.576333 0
12.272150 -16.595944 0
0 0 8 2 1
380.366 0.001165
28.5822 -0.026006
17.8892 0.166043
6.92862 -0.658914
1.78391 0.869336
0.843138 0.452132
0.205228 0.012973
0.076636 -0.002403
0 0 8 2 1
380.366 -0.000442
28.5822 0.005702
17.8892 -0.052894
6.92862 0.252087
1.78391 -0.470343
0.843138 -0.316144

0.205228 0.720625
0.076636 0.511114
0 0 1 0 1
0.205228 1
0 0 1 0 1
0.076636 1
0 2 6 6 1
18.5489 0.037021
9.56696 -0.193866
2.21861 0.657594
0.921459 0.455506
0.217858 0.027216
0.069320 -0.004604
0 2 6 2 1
18.5489 -0.009052
9.56696 0.051762
2.21861 -0.221743
0.921459 -0.124279
0.217858 0.521853
0.069320 0.609937
0 2 1 0 1
0.069320 1
0 3 6 10 1
38.5626 0.004261
21.7613 -0.006897
3.66111 0.276277
1.55833 0.514323
0.609523 0.344559
0.1897 0.051594
0 3 1 0 1
0.1897 1
252 6
input
6. 0 2 4 2 2 0
2.656483 50.217674 0
2.281974 1.982941 0
2.946988 39.938015 0
2.790001 79.873384 0
1.750168 -0.651126 0
1.909579 -1.288332 0
1.107233 5.059096 0
1.084059 7.498701 0
1.992613 -7.997183 0
1.968281 -10.464938 0
0 0 3 2 1

4.620870 -0.076259
3.407086 0.222163
1.353795 -0.541514
0 0 1 0 1
0.278218 1.0
0 0 1 0 1
0.128403 1.0
0 2 3 4 1
4.772823 -0.038412
3.508559 0.112992
1.653984 -0.229605
0 2 1 0 1
0.326880 1.0
0 2 1 0 1
0.139746 1.0
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

InAs

InAs – Phys Rev, Serie 3. B (1990) 41 12079
crystal
0 0 0
216
6.058
2
249 0. 0. 0.
233 0.25 0.25 0.25
printout
basisset
end
end
249 9
input
21. 0 2 4 4 2
15.392822 281.122350 0
8.055864 61.901470 0
13.928672 67.462154 0
13.347234 134.949250 0
7.614132 14.746140 0
7.318365 29.639262 0
14.034715 35.493254 0
14.511616 53.178773 0
5.550550 9.177281 0
5.059415 12.392410 0
12.539056 -13.728078 0
12.552561 -18.206866 0
0 0 8 2 1
265.131 0.000770
25.5694 -0.052791
16.0041 0.259343
6.81885 -0.739289
1.66676 0.885773
0.769232 0.442592
0.170415 0.011574
0.1 -0.002451
0 0 8 2 1
265.131 -0.000230
25.5694 0.014088
16.0041 -0.078615
6.81885 0.252864
1.66676 -0.415545
0.769232 -0.296647

0.170415 0.678578
0.1 0.527129
0 0 1 0 1
0.170415 1
0 0 1 0 1
0.1 1
0 2 6 6 1
14.4691 0.090177
9.28083 -0.267642
2.08201 0.664483
0.844314 0.461690
0.186900 0.027059
0.1 -0.004677
0 2 6 1 1
14.4691 -0.019023
9.28083 0.059157
2.08201 -0.180749
0.844314 -0.114582
0.186900 0.440739
0.1 0.687789
0 2 1 0 1
0.1 1
0 3 6 10 1
30.7879 0.005766
19.2555 -0.010708
3.19662 0.293860
1.33210 0.510869
0.504619 0.341519
0.1498 0.052465
0 3 1 0 1
0.1498 1
233 9
input
23. 0 2 4 6 2
28.725122 370.114025 0
6.767681 9.349296 0
45.331064 99.142103 0
44.767415 198.307880 0
19.539090 28.383073 0
18.973471 56.871464 0
51.057152 -18.485145 0
50.151340 -28.113530 0
16.108936 -1.223895 0
14.672223 -1.345765 0
3.851927 0.101757 0

3.813502 0.170338 0
11.940584 -0.775230 0
17.761160 -2.157259 0
0 0 8 2 1
2542.81 0.001137
381.169 0.006055
40.2342 0.084125
16.1217 -0.405285
3.20189 0.712926
1.42096 0.473376
0.321443 0.018013
0.116735 -0.003720
0 0 8 2 1
2542.81 -0.000390
381.169 -0.002190
40.2342 -0.026853
16.1217 0.136878
3.20189 -0.320457
1.42096 -0.337391
0.321443 0.676384
0.116735 0.534980
0 0 1 0 1
0.321443 1
0 0 1 0 1
0.116735 1
0 2 7 6 1
99.5349 0.003857
24.1195 -0.085101
5.84196 0.404762
2.56010 0.531478
1.09308 0.184012
0.318424 0.005764
0.100972 -0.000352
0 2 7 3 1
99.5349 -0.000772
24.1195 0.019941
5.84196 -0.107210
2.56010 -0.172259
1.09308 0.008761
0.318424 0.569744
0.100972 0.535653
0 2 1 0 1
0.100972 1
0 3 7 10 1
113.509 0.011980

36.8872 0.079544
13.6893 0.236755
5.38964 0.401534
2.08046 0.406686
0.737568 0.173162
0.3078 0.008730
0 3 1 0 1
0.3078 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.001
end

VO2

VO2 – Acta Chemica Scandinavica (1-27,1973-42,1988) (1956) 10, p623-p628
CRYSTAL
0 0 0
14
5.3480 4.5170 5.3750 115.235
3
223 0.2580 0.0250 0.2830
8 0.60 0.21 0.4
8 0.11 0.31 0.4
PRINTOUT
BASISSET
END
END
223 10
INPUT
13. 0 2 2 2 0 0
14.490000 178.447971 0
6.524000 19.831375 0
14.300000 109.529763 0
6.021000 12.570310 0
17.480000 -19.219657 0
5.709000 -0.642775 0
0 0 3 2 1
12.8432080 1.1406430
11.3757530 -1.2188030
5.4069740 -0.8929030
0 0 1 2 1
1.4659270 1.0
0 0 1 0 1
0.5980800 1.0
0 0 1 0 1
0.0887900 1.0
0 2 2 6 1
31.8898680 0.0394070
8.2371780 -1.0226030
0 2 2 0 1
4.3283730 0.1927560
1.5405260 0.8511680
0 2 1 0 1
0.5280810 1.0
0 2 1 0 1
0.0899620 1.0
0 3 4 3 1

22.6804330 0.0362930
6.8613120 0.1773010
2.2754450 0.4304290
0.7319220 0.5893030
0 3 1 0 1
0.2007460 1.0
8 4
0 0 6 2 1
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 6 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
END

InN

InN (wurtzite)– Powder Diffraction (2003) 18, p114-p121
crystal
0 0 0
186
3.5377 5.7037
2
249 0.3333 0.6667 0.0
7 0.3333 0.6667 0.3769
printout
basisset
end
end
249 9
input
21. 0 2 4 4 2
15.392822 281.122350 0
8.055864 61.901470 0
13.928672 67.462154 0
13.347234 134.949250 0
7.614132 14.746140 0
7.318365 29.639262 0
14.034715 35.493254 0
14.511616 53.178773 0
5.550550 9.177281 0
5.059415 12.392410 0
12.539056 -13.728078 0
12.552561 -18.206866 0
0 0 8 2 1
265.131 0.000770
25.5694 -0.052791
16.0041 0.259343
6.81885 -0.739289
1.66676 0.885773
0.769232 0.442592
0.170415 0.011574
0.1 -0.002451
0 0 8 2 1
265.131 -0.000230
25.5694 0.014088
16.0041 -0.078615
6.81885 0.252864
1.66676 -0.415545
0.769232 -0.296647

0.170415 0.678578
0.1 0.527129
0 0 1 0 1
0.170415 1
0 0 1 0 1
0.1 1
0 2 6 6 1
14.4691 0.090177
9.28083 -0.267642
2.08201 0.664483
0.844314 0.461690
0.186900 0.027059
0.1 -0.004677
0 2 6 1 1
14.4691 -0.019023
9.28083 0.059157
2.08201 -0.180749
0.844314 -0.114582
0.186900 0.440739
0.1 0.687789
0 2 1 0 1
0.1 1
0 3 6 10 1
30.7879 0.005766
19.2555 -0.010708
3.19662 0.293860
1.33210 0.510869
0.504619 0.341519
0.1498 0.052465
0 3 1 0 1
0.1498 1
7 5
0 0 6 2 1
6293.4800000 0.00196979
949.0440000 0.0149613
218.7760000 0.0735006
63.6916000 0.2489370
18.8282000 0.6024600
2.7202300 0.2562020
0 1 3 5 1
30.6331000 0.1119060 0.0383119
7.0261400 0.9216660 0.2374030
2.1120500 -0.00256919 0.8175920
0 1 1 0 1
0.6840090 1.0000000 1.0000000

0 1 1 0 1
0.2008780 1.0000000 1.0000000
0 3 1 0 1
0.9130000 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

Ge

Ge – Acta Crystallographica (1,1948-23,1967) (1962) 15, p578-p582
crystal
0 0 0
227
5.6568
1
232 0.1250 0.1250 0.1250
printout
basisset
end
end
232 9
input
22. 0 2 4 6 2
27.242225 370.236090 0
7.467948 9.214629 0
45.567991 99.135034 0
45.517505 198.271454 0
18.245769 28.388121 0
17.651078 56.803471 0
52.760598 -17.967085 0
53.136663 -26.815539 0
14.564079 -1.383893 0
12.631857 -2.072663 0
3.923042 0.080334 0
3.738774 0.238529 0
11.407378 -0.705680 0
18.429054 -2.475951 0
0 0 8 2 1
2611.74 0.000656
390.030 0.003595
34.2279 0.100126
15.1072 -0.434959
2.92774 0.735500
1.27159 0.458592
0.262497 0.015064
0.094306 -0.003504
0 0 8 2 1
2611.74 -0.000201
390.030 -0.001176
34.2279 -0.029187
15.1072 0.134027
2.92774 -0.295806

1.27159 -0.308730
0.262497 0.660266
0.094306 0.529644
0 0 1 0 1
0.262497 1
0 0 1 0 1
0.094306 1
0 2 7 6 1
108.379 0.002678
22.6697 -0.080763
5.36897 0.398676
2.36025 0.523026
1.00458 0.198456
0.260840 0.007404
0.1 -0.000728
0 2 7 2 1
108.379 -0.000461
22.6697 0.016658
5.36897 -0.091791
2.36025 -0.148559
1.00458 0.000308
0.260840 0.538550
0.1 0.571224
0 2 1 0 1
0.1 1
0 3 7 10 1
98.8248 0.013096
32.0078 0.081149
11.8456 0.243246
4.62772 0.401474
1.75844 0.402437
0.609192 0.178540
0.2425 0.010049
0 3 1 0 1
0.2425 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14

end
12 0 24
maxcycle
60
tolscf
7 7
fmixing
60
broyden
0.0001
end

GaSb

GaSb – Physical Review (1,1893-132,1963/141,1966-188,1969) (1954) 96, p576-p577
crystal
0 0 0
216
6.1347
2
231 0. 0. 0.
251 0.25 0.25 0.25
printout
basisset
end
end
231 9
input
21. 0 2 4 6 2 0
25.880361 370.273040 0
7.901295 9.190615 0
45.149190 99.144001 0
44.979981 198.295512 0
17.224251 28.445653 0
16.747329 56.949705 0
51.968812 -18.168797 0
51.629117 -27.380273 0
15.241738 -1.587022 0
15.320193 -2.516292 0
4.918589 0.083166 0
4.755103 0.202198 0
10.762263 -0.616990 0
19.852939 -3.138584 0
0 0 8 2 1
2848.20 0.000362
420.664 0.002117
29.8118 0.118964
14.2207 -0.461723
2.67643 0.751559
1.13353 0.447202
0.207220 0.012746
0.1 -0.003358
0 0 8 2 1
2848.20 -0.000097
420.664 -0.000614
29.8118 -0.031069
14.2207 0.126784

2.67643 -0.264288
1.13353 -0.275471
0.207220 0.633842
0.1 0.531681
0 0 1 0 1
0.207220 1
0 0 1 0 1
0.1 1
0 2 7 6 1
109.624 0.002101
21.0855 -0.080196
4.92260 0.396415
2.15591 0.519076
0.901913 0.207520
0.202004 0.007825
0.1 -0.001129
0 2 7 1 1
109.624 -0.000288
21.0855 0.013555
4.92260 -0.073629
2.15591 -0.120860
0.901913 -0.001960
0.202004 0.493206
0.1 0.620604
0 2 1 0 1
0.1 1
0 3 7 10 1
85.7978 0.014668
27.6822 0.085621
10.1760 0.248336
3.92208 0.401414
1.45858 0.398604
0.488760 0.186898
0.1772 0.012331
0 3 1 0 1
0.1772 1
251 9
input
23. 0 2 4 4 2 0
16.330865 281.071581 0
8.556542 61.716604 0
14.470337 67.457380 0
13.816194 134.933503 0
8.424924 14.716344 0
8.092728 29.518512 0

14.886331 35.447815 0
15.146319 53.143466 0
5.908267 9.179223 0
5.594322 13.240253 0
14.444978 -15.366801 0
14.449295 -20.296138 0
0 0 8 2. 1
371.584 0.001591
26.5392 -0.041684
16.6213 0.273343
7.73551 -0.767685
1.89234 0.899496
0.910431 0.431387
0.244231 0.012837
0.092397 -0.002173
0 0 8 2. 1
371.584 0.000654
26.5392 -0.010962
16.6213 0.093833
7.73551 -0.304009
1.89234 0.508409
0.910431 0.339239
0.244231 -0.734772
0.092397 -0.526134
0 0 1 0. 1
0.244231 1
0 0 1 0. 1
0.092397 1
0 2 6 6. 1
16.0509 0.092157
10.2621 -0.275559
2.42832 0.65864
1.03360 0.466892
0.25944 0.028511
0.086108 -0.005155
0 2 6 3. 1
16.0509 -0.025313
10.2621 0.079796
2.42832 -0.242094
1.03360 -0.148605
0.25944 0.548944
0.086108 0.589291
0 2 1 0. 1
0.086108 1
0 3 6 10. 1

45.4785 0.003259
18.5114 -0.005497
3.91600 0.279953
1.71482 0.512751
0.697319 0.332872
0.2304 0.048843
0 3 1 0. 1
0.2304 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
60
tolscf
7 7
fmixing
60
broyden
0.0001
end

SnSe

SnSe – Physica B, Condensed Matter (2012) 407, (21) p4154-p4159
crystal
0 0 0
62
11.5000 4.1540 4.4460
2
250 0.1180 0.2500 0.1043
234 0.3559 0.2500 0.0164
printout
basisset
end
end
250 5
input
4. 0 2 4 2 2 0
2.081778 67.925555 0
1.070042 -7.309665 0
2.094274 18.867005 0
2.020067 37.732449 0
0.998866 -0.725179 0
1.095504 -1.466610 0
0.754006 2.602362 0
0.741783 3.923355 0
1.231292 -4.332527 0
1.229112 -5.776780 0
0 0 3 2 1
1.564000 0.809442
1.147943 -1.641437
0.844112 0.489837
0 0 1 0 1
0.183681 1.0
0 0 1 0 1
0.079194 1.0
0 2 3 2 1
1.897761 0.127301
1.405749 -0.245617
0.260882 0.290765
0 2 1 0 1
0.1 1.0
234 9
input
24. 0 2 4 6 2 0
30.046990 370.122888 0

6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1
0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1
100.0192 -0.001058

25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

Si

Si– Materials Science Forum (2001) 378, p288-p293
CRYSTAL
0 0 0
227
5.4305
1
14 0.1250 0.1250 0.1250
PRINTOUT
BASISSET
END
END
14 12
0 0 6 2 1
69379.2300000 0.0007570
10354.9400000 0.0059320
2333.8796000 0.0310880
657.1429500 0.1249670
214.3011300 0.3868970
77.6291680 0.5548880
0 0 3 2 1
77.6291680 0.1778810
30.6308070 0.6277650
12.8012950 0.2476230
0 0 1 2 1
3.9268660 1.0000000
0 0 1 0 1
1.4523430 1.0000000
0 0 1 0 1
0.2562340 1.0000000
0 0 1 0 1
0.1 1.0000000
0 2 4 6 1
335.4831900 0.0088660
78.9003660 0.0682990
24.9881500 0.2909580
9.2197110 0.7321170
0 2 2 2 1
3.6211400 0.6198790
1.4513100 0.4391480
0 2 1 0 1
0.5049770 1.0000000
0 2 1 0 1
0.1863170 1.0000000

0 2 1 0 1
0.1 1.0000000
0 3 1 0 1
0.4500000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

MoS2

MOS2 – Zeitschrift fuer Anorganische und Allgemeine Chemie (1950) (DE) (1986) 540, p15-p17
crystal
0 0 0
194
3.1602 12.2940
2
242 0.33333333 0.66666667 0.2500
16 0.33333333 0.66666667 0.6210
printout
basisset
end
end
242 10
input
14. 0 2 4 4 2 0
10.097000 180.076853 0
4.375670 24.715920 0
9.126564 41.227678 0
8.863223 82.452670 0
4.044948 6.345092 0
3.866657 12.458423 0
7.535754 19.308744 0
7.278976 28.977674 0
2.763205 3.189516 0
2.772085 4.700169 0
6.306633 -7.178888 0
6.356448 -9.745978 0
0 0 6 2 1
0.10697800E+03 0.73500000E-03
0.18882400E+02 -0.35090000E-01
0.11807700E+02 0.14734800E+00
0.40211800E+01 -0.58336300E+00
0.95681600E+00 0.82563500E+00
0.43569200E+00 0.45231100E+00
0 0 6 2 1
0.10697800E+03 -0.17600000E-03
0.18882400E+02 0.93320000E-02
0.11807700E+02 -0.43811000E-01
0.40211800E+01 0.19723200E+00
0.95681600E+00 -0.37731100E+00
0.43569200E+00 -0.29396700E+00
0 0 6 0 1

0.10697800E+03 0.11660000E-02
0.18882400E+02 -0.37607000E-01
0.11807700E+02 0.12598000E+00
0.40211800E+01 -0.47523700E+00
0.95681600E+00 0.14989830E+01
0.43569200E+00 -0.82234500E+00
0 0 1 0 1
0.12 0.10000000E+01
0 2 5 6 1
0.11411800E+02 0.25345000E-01
0.52453500E+01 -0.17521300E+00
0.13188400E+01 0.48127200E+00
0.62298300E+00 0.49726100E+00
0.27910800E+00 0.15955500E+00
0 2 5 0 1
0.11411800E+02 -0.70220000E-02
0.52453500E+01 0.53339000E-01
0.13188400E+01 -0.17564300E+00
0.62298300E+00 -0.21621300E+00
0.27910800E+00 0.67958000E-01
0 2 1 0 1
0.12 0.10000000E+01
0 3 5 4 1
0.52576100E+01 -0.14761000E-01
0.21046200E+01 0.13198200E+00
0.95820100E+00 0.34708600E+00
0.41404700E+00 0.40547100E+00
0.16845000E+00 0.28805800E+00
0 3 5 0 1
0.52576100E+01 0.15439000E-01
0.21046200E+01 -0.16062100E+00
0.95820100E+00 -0.42322900E+00
0.41404700E+00 -0.19233900E+00
0.16845000E+00 0.53145900E+00
0 3 1 0 1
0.12 0.10000000E+01
16 12
0 0 6 2 1
93413.4000000 0.0007430
13961.7000000 0.0057930
3169.9100000 0.0299540
902.4560000 0.1190280
297.1580000 0.3684320
108.7020000 0.5772990
0 0 3 2 1

108.7020000 0.1431860
43.1553000 0.6244650
18.1079000 0.2833660
0 0 1 2 1
5.5600900 1.0000000
0 0 1 0 1
2.1318300 1.0000000
0 0 1 0 1
0.4204030 1.0000000
0 0 1 0 1
0.1360450 1.0000000
0 2 4 6 1
495.0400000 0.0083090
117.2210000 0.0640240
37.7749000 0.2776140
14.0584000 0.7450760
0 2 2 4 1
5.5657400 0.6137120
2.2629700 0.4438180
0 2 1 0 1
0.8079940 1.0000000
0 2 1 0 1
0.2774600 1.0000000
0 2 1 0 1
0.12 1.
0 3 1 0 1
0.6500000 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 9 30
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80

broyden
0.0001
end

InP

InP – Physical Review, Serie 3. B - Condensed Matter (18,1978-) (1990) 41, p12079-p12085
crystal
0 0 0
216
5.869
2
249 0. 0. 0.
15 0.25 0.25 0.25
printout
basisset
end
end
249 9
input
21. 0 2 4 4 2
15.392822 281.122350 0
8.055864 61.901470 0
13.928672 67.462154 0
13.347234 134.949250 0
7.614132 14.746140 0
7.318365 29.639262 0
14.034715 35.493254 0
14.511616 53.178773 0
5.550550 9.177281 0
5.059415 12.392410 0
12.539056 -13.728078 0
12.552561 -18.206866 0
0 0 8 2 1
265.131 0.000770
25.5694 -0.052791
16.0041 0.259343
6.81885 -0.739289
1.66676 0.885773
0.769232 0.442592
0.170415 0.011574
0.1 -0.002451
0 0 8 2 1
265.131 -0.000230
25.5694 0.014088
16.0041 -0.078615
6.81885 0.252864
1.66676 -0.415545
0.769232 -0.296647

0.170415 0.678578
0.1 0.527129
0 0 1 0 1
0.170415 1
0 0 1 0 1
0.1 1
0 2 6 6 1
14.4691 0.090177
9.28083 -0.267642
2.08201 0.664483
0.844314 0.461690
0.186900 0.027059
0.1 -0.004677
0 2 6 1 1
14.4691 -0.019023
9.28083 0.059157
2.08201 -0.180749
0.844314 -0.114582
0.186900 0.440739
0.1 0.687789
0 2 1 0 1
0.1 1
0 3 6 10 1
30.7879 0.005766
19.2555 -0.010708
3.19662 0.293860
1.33210 0.510869
0.504619 0.341519
0.1498 0.052465
0 3 1 0 1
0.1498 1
15 12
0 0 6 2 1
77492.4000000 0.0007810
11605.8000000 0.0060680
2645.9600000 0.0311600
754.9760000 0.1234310
248.7550000 0.3782090
91.1565000 0.5632620
0 0 3 2 1
91.1565000 0.1602550
36.2257000 0.6276470
15.2113000 0.2638490
0 0 1 2 1
4.7941700 1.0000000

0 0 1 0 1
1.8079300 1.0000000
0 0 1 0 1
0.3568160 1.0000000
0 0 1 0 1
0.1147830 1.0000000
0 2 4 6 1
384.8430000 0.0092060
90.5521000 0.0698740
29.1339000 0.2924700
10.8862000 0.7281030
0 2 2 3 1
4.3525900 0.6283490
1.7770600 0.4280440
0 2 1 0 1
0.6970050 1.0000000
0 2 1 0 1
0.2535320 1.0000000
0 2 1 0 1
0.1 1.0000000
0 3 1 0 1
0.5500000 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.01
end

GaAs

GaAs – Acta Crystallographica. Section A: Foundations of Crystallography (1994) 50, p621-p632
crystal
0 0 0
216
5.6521
2
231 0. 0. 0.
233 0.25 0.25 0.25
printout
basisset
end
end
231 9
input
21. 0 2 4 6 2 0
25.880361 370.273040 0
7.901295 9.190615 0
45.149190 99.144001 0
44.979981 198.295512 0
17.224251 28.445653 0
16.747329 56.949705 0
51.968812 -18.168797 0
51.629117 -27.380273 0
15.241738 -1.587022 0
15.320193 -2.516292 0
4.918589 0.083166 0
4.755103 0.202198 0
10.762263 -0.616990 0
19.852939 -3.138584 0
0 0 8 2 1
2848.20 0.000362
420.664 0.002117
29.8118 0.118964
14.2207 -0.461723
2.67643 0.751559
1.13353 0.447202
0.207220 0.012746
0.1 -0.003358
0 0 8 2 1
2848.20 -0.000097
420.664 -0.000614
29.8118 -0.031069

14.2207 0.126784
2.67643 -0.264288
1.13353 -0.275471
0.207220 0.633842
0.1 0.531681
0 0 1 0 1
0.207220 1
0 0 1 0 1
0.1 1
0 2 7 6 1
109.624 0.002101
21.0855 -0.080196
4.92260 0.396415
2.15591 0.519076
0.901913 0.207520
0.202004 0.007825
0.1 -0.001129
0 2 7 1 1
109.624 -0.000288
21.0855 0.013555
4.92260 -0.073629
2.15591 -0.120860
0.901913 -0.001960
0.202004 0.493206
0.1 0.620604
0 2 1 0 1
0.1 1
0 3 7 10 1
85.7978 0.014668
27.6822 0.085621
10.1760 0.248336
3.92208 0.401414
1.45858 0.398604
0.488760 0.186898
0.1772 0.012331
0 3 1 0 1
0.1772 1
233 9
input
23. 0 2 4 6 2
28.725122 370.114025 0
6.767681 9.349296 0
45.331064 99.142103 0
44.767415 198.307880 0
19.539090 28.383073 0

18.973471 56.871464 0
51.057152 -18.485145 0
50.151340 -28.113530 0
16.108936 -1.223895 0
14.672223 -1.345765 0
3.851927 0.101757 0
3.813502 0.170338 0
11.940584 -0.775230 0
17.761160 -2.157259 0
0 0 8 2 1
2542.81 0.001137
381.169 0.006055
40.2342 0.084125
16.1217 -0.405285
3.20189 0.712926
1.42096 0.473376
0.321443 0.018013
0.116735 -0.003720
0 0 8 2 1
2542.81 -0.000390
381.169 -0.002190
40.2342 -0.026853
16.1217 0.136878
3.20189 -0.320457
1.42096 -0.337391
0.321443 0.676384
0.116735 0.534980
0 0 1 0 1
0.321443 1
0 0 1 0 1
0.116735 1
0 2 7 6 1
99.5349 0.003857
24.1195 -0.085101
5.84196 0.404762
2.56010 0.531478
1.09308 0.184012
0.318424 0.005764
0.100972 -0.000352
0 2 7 3 1
99.5349 -0.000772
24.1195 0.019941
5.84196 -0.107210
2.56010 -0.172259
1.09308 0.008761

0.318424 0.569744
0.100972 0.535653
0 2 1 0 1
0.100972 1
0 3 7 10 1
113.509 0.011980
36.8872 0.079544
13.6893 0.236755
5.38964 0.401534
2.08046 0.406686
0.737568 0.173162
0.3078 0.008730
0 3 1 0 1
0.3078 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.01
end

CdTe

CdTe – Kristallografiya (2001) 46, (4) p703-p709
crystal
0 0 0
216
6.4827
2
248 0.000 0.000 0.000
252 0.25 0.25 0.25
printout
basisset
end
end
248 10
input
20. 0 2 4 4 2 0
13.355176 270.039448 0
7.308378 38.877766 0
12.659728 64.607470 0
12.289639 129.219445 0
6.786176 10.622558 0
6.400743 21.265046 0
11.161722 31.663965 0
11.219615 47.489216 0
4.537733 5.186200 0
4.335727 7.566063 0
11.478986 -12.632785 0
11.487027 -16.760171 0
0 0 7 2 1
0.22385300e+03 0.87100000e-03
0.23094800e+02 -0.64307000e-01
0.14652200e+02 0.30131600e+00
0.65704440e+01 -0.76052400e+00
0.15378300e+01 0.89407100e+00
0.69098400e+00 0.42787900e+00
0.13491300e+00 0.10188000e-01
0 0 7 2 1
0.22385300e+03 -0.22900000e-03
0.23094800e+02 0.15594000e-01
0.14652200e+02 -0.81047000e-01
0.65704440e+01 0.22725100e+00
0.15378300e+01 -0.36256300e+00
0.69098400e+00 -0.25078300e+00
0.13491300e+00 0.61353300e+00

0 0 7 0 1
0.22385300e+03 0.10770000e-02
0.23094800e+02 -0.71649000e-01
0.14652200e+02 0.28897500e+00
0.65704440e+01 -0.73154600e+00
0.15378300e+01 0.19768990e+01
0.69098400e+00 -0.13519510e+01
0.13491300e+00 -0.11186740e+01
0 0 1 0 1
0.07 0.10000000e+01
0 2 6 6 1
0.13717500e+02 0.77616000e-01
0.84632200e+01 -0.25794300e+00
0.21182000e+01 0.53527400e+00
0.98926200e+00 0.49636200e+00
0.43178100e+00 0.12310900e+00
0.13916000e+00 0.32100000e-02
0 2 6 0 1
0.13717500e+02 -0.30730000e-01
0.84632200e+01 0.10874400e+00
0.21182000e+01 -0.27823100e+00
0.98926200e+00 -0.32939000e+00
0.43178100e+00 0.35463000e+00
0.13916000e+00 0.78145800e+00
0 2 1 0 1
0.09 0.10000000e+01
0 3 6 10 1
0.31669700e+02 0.31630000e-02
0.12221400e+02 -0.11791000e-01
0.31219900e+01 0.24119400e+00
0.13894100e+01 0.44899800e+00
0.57320300e+00 0.38021100e+00
0.21170800e+00 0.14455300e+00
0 3 6 0 1
0.31669700e+02 -0.48710000e-02
0.12221400e+02 0.18582000e-01
0.31219900e+01 -0.47667300e+00
0.13894100e+01 -0.45760400e+00
0.57320300e+00 0.57146200e+00
0.21170800e+00 0.49738000e+00
0 3 1 0 1
0.21170800e+00 0.10000000e+01
252 9
input
24. 0 2 4 4 2 0

16.814473 281.045843 0
8.793526 61.620656 0
14.877801 67.449464 0
14.269731 134.904304 0
8.724435 14.689547 0
8.291515 29.415063 0
15.205008 35.432057 0
15.225848 53.135687 0
6.071769 9.069802 0
5.804760 13.122304 0
15.206168 -15.745450 0
15.201702 -20.742448 0
0 0 8 2. 1
2111.19 0.000612
311.691 0.003207
13.8226 0.405512
8.71748 -0.932588
1.98303 0.919657
0.970377 0.404671
0.279765 0.012366
0.106776 -0.001604
0 0 8 2. 1
2111.19 0.000251
311.691 0.001457
13.8226 0.163702
8.71748 -0.398455
1.98303 0.578074
0.970377 0.327124
0.279765 -0.784654
0.106776 -0.499451
0 0 1 0. 1
0.279765 1
0 0 1 0. 1
0.106776 1
0 2 6 6. 1
17.0629 0.089340
10.8306 -0.271168
2.59380 0.662023
1.12676 0.460744
0.300176 0.028809
0.097551 -0.003863
0 2 6 4. 1
17.0629 -0.026861
10.8306 0.086304
2.59380 -0.273502

1.12676 -0.151390
0.300176 0.583976
0.097551 0.565014
0 2 1 0. 1
0.097551 1
0 3 6 10. 1
50.9106 0.003354
18.4647 -0.003642
4.27617 0.278080
1.89770 0.516348
0.786480 0.326571
0.2638 0.045152
0 3 1 0. 1
0.2638 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

AlSb

AlSb – Physical Review (1,1893-132,1963/141,1966-188,1969) (1954) 96, p578-p580
crystal
0 0 0
216
6.0959
2
13 0. 0. 0.
251 0.25 0.25 0.25
printout
basisset
end
end
13 5
0 0 6 2 1
13983.1000000 0.00194267
2098.7500000 0.0148599
477.7050000 0.0728494
134.3600000 0.2468300
42.8709000 0.4872580
14.5189000 0.3234960
0 1 6 8 1
239.6680000 -0.00292619 0.00460285
57.4419000 -0.0374080 0.0331990
18.2859000 -0.1144870 0.1362820
6.5991400 0.1156350 0.3304760
2.4904900 0.6125950 0.4491460
0.9445400 0.3937990 0.2657040
0 1 1 0 1
0.1 1. 1.
0 1 3 3 1
1.2779000 -0.2276060 -0.0175130
0.3975900 0.00144583 0.2445330
0.1600950 1.0927900 0.8049340
0 3 1 0 1
0.325 1.0
251 9
input
23. 0 2 4 4 2 0
16.330865 281.071581 0
8.556542 61.716604 0
14.470337 67.457380 0
13.816194 134.933503 0
8.424924 14.716344 0

8.092728 29.518512 0
14.886331 35.447815 0
15.146319 53.143466 0
5.908267 9.179223 0
5.594322 13.240253 0
14.444978 -15.366801 0
14.449295 -20.296138 0
0 0 8 2. 1
371.584 0.001591
26.5392 -0.041684
16.6213 0.273343
7.73551 -0.767685
1.89234 0.899496
0.910431 0.431387
0.244231 0.012837
0.092397 -0.002173
0 0 8 2. 1
371.584 0.000654
26.5392 -0.010962
16.6213 0.093833
7.73551 -0.304009
1.89234 0.508409
0.910431 0.339239
0.244231 -0.734772
0.092397 -0.526134
0 0 1 0. 1
0.244231 1
0 0 1 0. 1
0.092397 1
0 2 6 6. 1
16.0509 0.092157
10.2621 -0.275559
2.42832 0.65864
1.03360 0.466892
0.25944 0.028511
0.086108 -0.005155
0 2 6 3. 1
16.0509 -0.025313
10.2621 0.079796
2.42832 -0.242094
1.03360 -0.148605
0.25944 0.548944
0.086108 0.589291
0 2 1 0. 1
0.086108 1

0 3 6 10. 1
45.4785 0.003259
18.5114 -0.005497
3.91600 0.279953
1.71482 0.512751
0.697319 0.332872
0.2304 0.048843
0 3 1 0. 1
0.2304 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
60
tolscf
7 7
fmixing
60
broyden
0.0001
end

CdSe

CdSe – Phys Rev B (1993) 48, p11701-p11704
crystal
0 0 0
216
6.0770
2
248 0.000 0.000 0.000
234 0.25 0.25 0.25
printout
basisset
end
end
248 10
input
20. 0 2 4 4 2 0
13.355176 270.039448 0
7.308378 38.877766 0
12.659728 64.607470 0
12.289639 129.219445 0
6.786176 10.622558 0
6.400743 21.265046 0
11.161722 31.663965 0
11.219615 47.489216 0
4.537733 5.186200 0
4.335727 7.566063 0
11.478986 -12.632785 0
11.487027 -16.760171 0
0 0 7 2 1
0.22385300e+03 0.87100000e-03
0.23094800e+02 -0.64307000e-01
0.14652200e+02 0.30131600e+00
0.65704440e+01 -0.76052400e+00
0.15378300e+01 0.89407100e+00
0.69098400e+00 0.42787900e+00
0.13491300e+00 0.10188000e-01
0 0 7 2 1
0.22385300e+03 -0.22900000e-03
0.23094800e+02 0.15594000e-01
0.14652200e+02 -0.81047000e-01
0.65704440e+01 0.22725100e+00
0.15378300e+01 -0.36256300e+00
0.69098400e+00 -0.25078300e+00
0.13491300e+00 0.61353300e+00

0 0 7 0 1
0.22385300e+03 0.10770000e-02
0.23094800e+02 -0.71649000e-01
0.14652200e+02 0.28897500e+00
0.65704440e+01 -0.73154600e+00
0.15378300e+01 0.19768990e+01
0.69098400e+00 -0.13519510e+01
0.13491300e+00 -0.11186740e+01
0 0 1 0 1
0.07 0.10000000e+01
0 2 6 6 1
0.13717500e+02 0.77616000e-01
0.84632200e+01 -0.25794300e+00
0.21182000e+01 0.53527400e+00
0.98926200e+00 0.49636200e+00
0.43178100e+00 0.12310900e+00
0.13916000e+00 0.32100000e-02
0 2 6 0 1
0.13717500e+02 -0.30730000e-01
0.84632200e+01 0.10874400e+00
0.21182000e+01 -0.27823100e+00
0.98926200e+00 -0.32939000e+00
0.43178100e+00 0.35463000e+00
0.13916000e+00 0.78145800e+00
0 2 1 0 1
0.09 0.10000000e+01
0 3 6 10 1
0.31669700e+02 0.31630000e-02
0.12221400e+02 -0.11791000e-01
0.31219900e+01 0.24119400e+00
0.13894100e+01 0.44899800e+00
0.57320300e+00 0.38021100e+00
0.21170800e+00 0.14455300e+00
0 3 6 0 1
0.31669700e+02 -0.48710000e-02
0.12221400e+02 0.18582000e-01
0.31219900e+01 -0.47667300e+00
0.13894100e+01 -0.45760400e+00
0.57320300e+00 0.57146200e+00
0.21170800e+00 0.49738000e+00
0 3 1 0 1
0.21170800e+00 0.10000000e+01
234 9
input
24. 0 2 4 6 2

30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1
0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1

100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 7 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0.3656 0.007754
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

BP

BP – Congres International de Chimie pure et applique, 16eme Paris 1957, Mem. Sect. (1958) 1957, p539-p540
CRYSTAL
0 0 0
216
4.538
2
5 0.0000 0.0000 0.0000
15 0.25 0.25 0.25
PRINTOUT
BASISSET
END
END
5 5
0 0 6 2 1
2858.8900000 0.00215375
428.1400000 0.0165823
97.5282000 0.0821870
27.9693000 0.2766180
8.2157700 0.6293160
1.1127800 0.1737700
0 1 3 3 1
13.2415000 0.1174430 0.0418100
3.0016600 0.9180020 0.2365750
0.9128560 -0.00265105 0.8162140
0 1 1 0 1
0.3154540 1.0000000 1.0000000
0 1 1 0 1
0.1 1.0000000 1.0000000
0 3 1 0 1
0.4010000 1.0000000
15 12
0 0 6 2 1
77492.4000000 0.0007810
11605.8000000 0.0060680
2645.9600000 0.0311600
754.9760000 0.1234310
248.7550000 0.3782090
91.1565000 0.5632620
0 0 3 2 1
91.1565000 0.1602550
36.2257000 0.6276470
15.2113000 0.2638490

0 0 1 2 1
4.7941700 1.0000000
0 0 1 0 1
1.8079300 1.0000000
0 0 1 0 1
0.3568160 1.0000000
0 0 1 0 1
0.1147830 1.0000000
0 2 4 6 1
384.8430000 0.0092060
90.5521000 0.0698740
29.1339000 0.2924700
10.8862000 0.7281030
0 2 2 3 1
4.3525900 0.6283490
1.7770600 0.4280440
0 2 1 0 1
0.6970050 1.0000000
0 2 1 0 1
0.2535320 1.0000000
0 2 1 0 1
0.1 1.0000000
0 3 1 0 1
0.5500000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 9 30
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60

ANDERSON
PPAN
NODIRECT
END

Cu_2O

Cu2O – Journal of Solid State Chemistry (2006) 179, (2) p563-p572
crystal
0 0 0
224
4.2676
2
229 0.00 0.00 0.00
8 0.25 0.25 0.25
printout
basisset
end
end
229 10
input
19. 0 2 4 4 2 0
30.110543 355.750512 0
13.076310 70.930906 0
32.692614 77.969931 0
32.770339 155.927448 0
13.751067 18.021132 0
13.322166 36.094372 0
38.996511 -12.343410 0
39.539788 -18.273362 0
12.287511 -0.984705 0
11.459300 -1.318747 0
6.190102 -0.227264 0
8.118780 -0.468773 0
0 0 7 2 1
0.56008800e+03 0.63700000e-03
0.56648600e+02 -0.97350000e-02
0.35425800e+02 0.65793000e-01
0.11054600e+02 -0.41503500e+00
0.23068200e+01 0.74661100e+00
0.95142900e+00 0.46217300e+00
0.14518400e+00 0.15983000e-01
0 0 7 1 1
0.56008800e+03 -0.13600000e-03
0.56648600e+02 0.14010000e-02
0.35425800e+02 -0.13174000e-01
0.11054600e+02 0.95695000e-01
0.23068200e+01 -0.21187400e+00
0.95142900e+00 -0.23594400e+00
0.14518400e+00 0.50811500e+00

0 0 7 0 1
0.56008800e+03 -0.33300000e-03
0.56648600e+02 0.59300000e-02
0.35425800e+02 -0.32549000e-01
0.11054600e+02 0.21107100e+00
0.23068200e+01 -0.73055600e+00
0.95142900e+00 0.17724200e+00
0.14518400e+00 0.17148730e+01
0 0 1 0 1
0.12 0.10000000e+01
0 2 6 6 1
0.70973900e+02 0.36820000e-02
0.17851000e+02 -0.82128000e-01
0.42467900e+01 0.37537900e+00
0.18776000e+01 0.50840900e+00
0.79333500e+00 0.23909500e+00
0.19347600e+00 0.15850000e-01
0 2 6 0 1
0.70973900e+02 -0.62800000e-03
0.17851000e+02 0.16563000e-01
0.42467900e+01 -0.84572000e-01
0.18776000e+01 -0.14128300e+00
0.79333500e+00 -0.35710000e-02
0.19347600e+00 0.51900500e+00
0 2 1 0 1
0.12 0.10000000e+01
0 3 6 10 1
0.60380400e+02 0.17564000e-01
0.19112100e+02 0.99134000e-01
0.69528800e+01 0.27117100e+00
0.26099400e+01 0.40618000e+00
0.92256700e+00 0.38142700e+00
0.28364200e+00 0.20062600e+00
0 3 6 0 1
0.60380400e+02 -0.22286000e-01
0.19112100e+02 -0.12827400e+00
0.69528800e+01 -0.36279700e+00
0.26099400e+01 -0.32572200e+00
0.92256700e+00 0.32708700e+00
0.28364200e+00 0.65680900e+00
0 3 1 0 1
0.28364200e+00 0.10000000e+01
8 4
0 0 6 2 1
5484.6717000 0.0018311

825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 6 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

AlAs

AlAs – Physical Review, Serie 3. B - Condensed Matter (18,1978-) (1992) 46, (16) p10086-p10097
crystal
0 0 0
216
5.62
2
13 0. 0. 0.
233 0.25 0.25 0.25
printout
basisset
end
end
13 5
0 0 6 2 1
13983.1000000 0.00194267
2098.7500000 0.0148599
477.7050000 0.0728494
134.3600000 0.2468300
42.8709000 0.4872580
14.5189000 0.3234960
0 1 6 8 1
239.6680000 -0.00292619 0.00460285
57.4419000 -0.0374080 0.0331990
18.2859000 -0.1144870 0.1362820
6.5991400 0.1156350 0.3304760
2.4904900 0.6125950 0.4491460
0.9445400 0.3937990 0.2657040
0 1 1 0 1
0.1 1. 1.
0 1 3 3 1
1.2779000 -0.2276060 -0.0175130
0.3975900 0.00144583 0.2445330
0.1600950 1.0927900 0.8049340
0 3 1 0 1
0.325 1.0
233 9
input
23. 0 2 4 6 2
28.725122 370.114025 0
6.767681 9.349296 0
45.331064 99.142103 0
44.767415 198.307880 0

19.539090 28.383073 0
18.973471 56.871464 0
51.057152 -18.485145 0
50.151340 -28.113530 0
16.108936 -1.223895 0
14.672223 -1.345765 0
3.851927 0.101757 0
3.813502 0.170338 0
11.940584 -0.775230 0
17.761160 -2.157259 0
0 0 8 2 1
2542.81 0.001137
381.169 0.006055
40.2342 0.084125
16.1217 -0.405285
3.20189 0.712926
1.42096 0.473376
0.321443 0.018013
0.116735 -0.003720
0 0 8 2 1
2542.81 -0.000390
381.169 -0.002190
40.2342 -0.026853
16.1217 0.136878
3.20189 -0.320457
1.42096 -0.337391
0.321443 0.676384
0.116735 0.534980
0 0 1 0 1
0.321443 1
0 0 1 0 1
0.116735 1
0 2 7 6 1
99.5349 0.003857
24.1195 -0.085101
5.84196 0.404762
2.56010 0.531478
1.09308 0.184012
0.318424 0.005764
0.100972 -0.000352
0 2 7 3 1
99.5349 -0.000772
24.1195 0.019941
5.84196 -0.107210
2.56010 -0.172259

1.09308 0.008761
0.318424 0.569744
0.100972 0.535653
0 2 1 0 1
0.100972 1
0 3 7 10 1
113.509 0.011980
36.8872 0.079544
13.6893 0.236755
5.38964 0.401534
2.08046 0.406686
0.737568 0.173162
0.3078 0.008730
0 3 1 0 1
0.3078 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.01
end

GaP

GaP – Kristallografiya (1997) 42, p649-p659
crystal
0 0 0
216
5.448
2
231 0. 0. 0.
15 0.25 0.25 0.25
printout
basisset
end
end
231 9
input
21. 0 2 4 6 2 0
25.880361 370.273040 0
7.901295 9.190615 0
45.149190 99.144001 0
44.979981 198.295512 0
17.224251 28.445653 0
16.747329 56.949705 0
51.968812 -18.168797 0
51.629117 -27.380273 0
15.241738 -1.587022 0
15.320193 -2.516292 0
4.918589 0.083166 0
4.755103 0.202198 0
10.762263 -0.616990 0
19.852939 -3.138584 0
0 0 8 2 1
2848.20 0.000362
420.664 0.002117
29.8118 0.118964
14.2207 -0.461723
2.67643 0.751559
1.13353 0.447202
0.207220 0.012746
0.1 -0.003358
0 0 8 2 1
2848.20 -0.000097
420.664 -0.000614
29.8118 -0.031069
14.2207 0.126784

2.67643 -0.264288
1.13353 -0.275471
0.207220 0.633842
0.1 0.531681
0 0 1 0 1
0.207220 1
0 0 1 0 1
0.1 1
0 2 7 6 1
109.624 0.002101
21.0855 -0.080196
4.92260 0.396415
2.15591 0.519076
0.901913 0.207520
0.202004 0.007825
0.1 -0.001129
0 2 7 1 1
109.624 -0.000288
21.0855 0.013555
4.92260 -0.073629
2.15591 -0.120860
0.901913 -0.001960
0.202004 0.493206
0.1 0.620604
0 2 1 0 1
0.1 1
0 3 7 10 1
85.7978 0.014668
27.6822 0.085621
10.1760 0.248336
3.92208 0.401414
1.45858 0.398604
0.488760 0.186898
0.1772 0.012331
0 3 1 0 1
0.1772 1
15 12
0 0 6 2 1
77492.4000000 0.0007810
11605.8000000 0.0060680
2645.9600000 0.0311600
754.9760000 0.1234310
248.7550000 0.3782090
91.1565000 0.5632620
0 0 3 2 1

91.1565000 0.1602550
36.2257000 0.6276470
15.2113000 0.2638490
0 0 1 2 1
4.7941700 1.0000000
0 0 1 0 1
1.8079300 1.0000000
0 0 1 0 1
0.3568160 1.0000000
0 0 1 0 1
0.1147830 1.0000000
0 2 4 6 1
384.8430000 0.0092060
90.5521000 0.0698740
29.1339000 0.2924700
10.8862000 0.7281030
0 2 2 3 1
4.3525900 0.6283490
1.7770600 0.4280440
0 2 1 0 1
0.6970050 1.0000000
0 2 1 0 1
0.2535320 1.0000000
0 2 1 0 1
0.1 1.0000000
0 3 1 0 1
0.5500000 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80

broyden
0.01
end

ZnTe

ZnTe – Kristallografiya (1995) 40, (3) p505-p510
crystal
0 0 0
216
6.1060
2
230 0.000 0.000 0.000
252 0.25 0.25 0.25
printout
basisset
end
end
230 10
input
20. 0 2 4 4 2 0
34.174001 399.986399 0
14.456371 85.489750 0
39.888683 92.381077 0
39.655017 184.771176 0
15.290546 23.002541 0
14.903524 46.057427 0
43.708296 -13.690734 0
43.698536 -20.543980 0
15.150718 -1.316154 0
15.282441 -1.838715 0
8.160014 -0.370360 0
12.228422 -1.062943 0
0 0 7 2 1
0.62912600e+03 0.55900000e-03
0.62963500e+02 -0.96800000e-02
0.39579100e+02 0.62354000e-01
0.11917300e+02 -0.41487900e+00
0.25082400e+01 0.75446600e+00
0.10301900e+01 0.45899600e+00
0.15400200e+00 0.11664000e-01
0 0 7 2 1
0.62912600e+03 -0.12100000e-03
0.62963500e+02 0.14890000e-02
0.39579100e+02 -0.12737000e-01
0.11917300e+02 0.97246000e-01
0.25082400e+01 -0.21991700e+00
0.10301900e+01 -0.23647400e+00
0.15400200e+00 0.58129100e+00

0 0 7 0 1
0.62912600e+03 0.42100000e-03
0.62963500e+02 -0.51090000e-02
0.39579100e+02 0.41447000e-01
0.11917300e+02 -0.34164300e+00
0.25082400e+01 0.14386170e+01
0.10301900e+01 -0.98242900e+00
0.15400200e+00 -0.11876310e+01
0 0 1 0 1
0.1 0.10000000e+01
0 2 6 6 1
0.92903400e+02 0.24880000e-02
0.19745200e+02 -0.79136000e-01
0.45507300e+01 0.38805900e+00
0.20019000e+01 0.50935400e+00
0.84387900e+00 0.22457500e+00
0.20338100e+00 0.12680000e-01
0 2 6 0 1
0.92903400e+02 -0.53000000e-03
0.19745200e+02 0.24743000e-01
0.45507300e+01 -0.14247800e+00
0.20019000e+01 -0.23403200e+00
0.84387900e+00 0.92187000e-01
0.20338100e+00 0.83777000e+00
0 2 1 0 1
0.59572000e-01 0.10000000e+01
0 3 6 10 1
0.71276600e+02 0.15895000e-01
0.22760400e+02 0.92454000e-01
0.83236900e+01 0.25947200e+00
0.31687500e+01 0.40331400e+00
0.11470300e+01 0.38783400e+00
0.36664300e+00 0.20225800e+00
0 3 6 0 1
0.71276600e+02 -0.22516000e-01
0.22760400e+02 -0.13330300e+00
0.83236900e+01 -0.39325300e+00
0.31687500e+01 -0.35121400e+00
0.11470300e+01 0.40617100e+00
0.36664300e+00 0.57920500e+00
0 3 1 0 1
0.36664300e+00 0.10000000e+01
252 6
input
6. 0 2 4 2 2 0

2.656483 50.217674 0
2.281974 1.982941 0
2.946988 39.938015 0
2.790001 79.873384 0
1.750168 -0.651126 0
1.909579 -1.288332 0
1.107233 5.059096 0
1.084059 7.498701 0
1.992613 -7.997183 0
1.968281 -10.464938 0
0 0 3 2 1
4.620870 -0.076259
3.407086 0.222163
1.353795 -0.541514
0 0 1 0 1
0.278218 1.0
0 0 1 0 1
0.128403 1.0
0 2 3 4 1
4.772823 -0.038412
3.508559 0.112992
1.653984 -0.229605
0 2 1 0 1
0.326880 1.0
0 2 1 0 1
0.139746 1.0
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden

0.0001
end

FeO

FeO – Journal of Chemical Physics (1933) 1, p29-p36
CRYSTAL
0 0 0
225
4.3410
2
26 0. 0. 0.
8 0.5 0.5 0.5
PRINTOUT
BASISSET
END
SUPERCEL
0. 1. 1. 1. 0. 1. 1. 1. 0.
END
8 4
0 0 6 2 1
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 8 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
26 6
0 0 6 2 1
61132.6200000 1.766111E-03
9179.3420000 1.353038E-02
2090.8570000 6.673128E-02
589.2479000 2.314823E-01
188.7543000 4.797058E-01
64.4462900 3.501976E-01
0 1 6 8 1
1259.9800000 2.438014E-03 4.028019E-03
299.8761000 3.224048E-02 3.144647E-02
96.8491700 1.265724E-01 1.368317E-01
36.3102000 -3.139902E-02 3.487236E-01

14.7299600 -6.207593E-01 4.617931E-01
6.0660750 -4.502914E-01 2.043058E-01
0 1 6 8 1
50.4348500 -3.873256E-03 -7.017128E-03
16.8392900 7.196598E-02 -2.877660E-02
7.1920860 2.556591E-01 6.181383E-02
3.0534200 -2.882837E-01 3.954946E-01
1.2736430 -7.342822E-01 4.989059E-01
0.5040910 -2.049353E-01 1.791251E-01
0 1 3 1 1
1.9503160 0.05694869 -0.4593796
0.7367210 0.2882915 0.2852139
0.1141770 -1.1381590 0.9076485
0 3 3 5 1
23.1499400 8.876935E-02
6.1223680 3.896319E-01
1.8466010 7.014816E-01
0 3 1 0 1
0.5043610 1.00
99 0
END
UHF
DFT
B3PW
END
SHRINK
16 24
TOLINTEG
7 7 7 7 14
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
TOLDEE
7
MAXCYCLE
100
FMIXING
60
ANDERSON
PPAN
GUESSP
END

BiVO4

BiVO4 – Wu Li Hsueh Pao (= Acta Physica Sinica) (1983) 32, p1053-p1060
crystal
0 0 0
15
7.2532 11.7020 5.0960 134.234
4
283 0.0000 0.6337 0.2500
223 0.0000 0.1352 0.2500
8 0.1490 0.2100 0.1430
8 0.2580 0.4510 0.3790
printout
basisset
end
end
283 9
input
23. 0 2 4 4 2
13.043090 283.264227 0
8.221682 62.471959 0
10.467777 72.001499 0
9.118901 144.002277 0
6.754791 5.007945 0
6.252592 9.991550 0
8.081474 36.396259 0
7.890595 54.597664 0
4.955556 9.984294 0
4.704559 14.981485 0
4.214546 13.713383 0
4.133400 18.194308 0
0 0 8 2 1
211.821 0.001088
21.3262 -0.105862
13.3654 0.530808
6.94610 -1.050265
1.71229 0.995856
0.839107 0.398952
0.255364 0.011778
0.096700 -0.001470
0 0 8 2 1
211.821 0.000422
21.3262 -0.038537
13.3654 0.217238
6.94610 -0.481097

1.71229 0.701595
0.839107 0.290520
0.255364 -0.799778
0.096700 -0.496131
0 0 1 0 1
0.255364 1
0 0 1 0 1
0.096700 1
0 2 6 6 1
11.0644 0.167249
7.45000 -0.425262
2.01069 0.692525
0.888321 0.475374
0.236369 0.029859
0.079290 -0.004493
0 2 6 3 1
11.0644 -0.052201
7.45000 0.139083
2.01069 -0.293556
0.888321 -0.158574
0.236369 0.574362
0.079290 0.572678
0 2 1 0 1
0.079290 1
0 3 6 10 1
16.2461 0.007808
6.98363 -0.066831
2.37476 0.324140
1.15372 0.485831
0.525974 0.301056
0.2151 0.063196
0 3 1 0 1
0.2151 1
223 10
input
13. 0 2 2 2 0
14.490000 178.447971 0
6.524000 19.831375 0
14.300000 109.529763 0
6.021000 12.570310 0
17.480000 -19.219657 0
5.709000 -0.642775 0
0 0 3 2 1
12.8432080 1.1406430
11.3757530 -1.2188030

5.4069740 -0.8929030
0 0 1 2 1
1.4659270 1.0
0 0 1 0 1
0.5980800 1.0
0 0 1 0 1
0.0887900 1.0
0 2 2 6 1
31.8898680 0.0394070
8.2371780 -1.0226030
0 2 2 0 1
4.3283730 0.1927560
1.5405260 0.8511680
0 2 1 0 1
0.5280810 1.0
0 2 1 0 1
0.0899620 1.0
0 3 4 3 1
22.6804330 0.0362930
6.8613120 0.1773010
2.2754450 0.4304290
0.7319220 0.5893030
0 3 1 0 1
0.2007460 1.0
8 4
0 0 6 2 1
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 6 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
99 0
end
uhf
dft
b3pw

```
end
biesplit
10
tolinteg
7 7 7 7 14
end
6 0 12
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end
```

SiC (3C)

SiC (zb)– Journal of Materials Science (1986) 21, p4366-p4368
CRYSTAL
0 0 0
216
4.3581
2
14 0 0 0
6 0.250 0.250 0.250
PRINTOUT
BASISSET
END
END
14 5
0 0 6 2 1
16115.9000000 0.00195948
2425.5800000 0.01492880
553.8670000 0.07284780
156.3400000 0.24613000
50.0683000 0.48591400
17.0178000 0.32500200
0 1 6 8 1
292.7180000 -0.00278094 0.00443826
69.8731000 -0.03571460 0.03266790
22.3363000 -0.11498500 0.13472100
8.1503900 0.09356340 0.32867800
3.1345800 0.60301700 0.44964000
1.2254300 0.41895900 0.26137200
0 1 3 4 1
1.7273800 -0.24463000 -0.01779510
0.5729220 0.00431572 0.25353900
0.2221920 1.09818000 0.80066900
0 1 1 0 1
0.12 1.00000000 1.00000000
0 3 1 0 1
0.4500000 1.0000000
6 5
0 0 6 2 1
4563.2400000 0.00196665
682.0240000 0.0152306
154.9730000 0.0761269
44.4553000 0.2608010
13.0290000 0.6164620
1.8277300 0.2210060

0 1 3 4 1
20.9642000 0.1146600 0.0402487
4.8033100 0.9199990 0.2375940
1.4593300 -0.00303068 0.8158540
0 1 1 0 1
0.4834560 1.0000000 1.0000000
0 1 1 0 1
0.1455850 1.0000000 1.0000000
0 3 1 0 1
0.6260000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
20
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

AlP

AlP– Physical Review, Serie 3. B - Condensed Matter (18,1978-) (1992) 46, (16) p10086-p10097
CRYSTAL
0 0 0
216
5.4210
2
13 0.0000 0.0000 0.0000
15 0.2500 0.2500 0.2500
PRINTOUT
BASISSET
END
END
13 5
0 0 6 2 1
13983.1000000 0.00194267
2098.7500000 0.0148599
477.7050000 0.0728494
134.3600000 0.2468300
42.8709000 0.4872580
14.5189000 0.3234960
0 1 6 8 1
239.6680000 -0.00292619 0.00460285
57.4419000 -0.0374080 0.0331990
18.2859000 -0.1144870 0.1362820
6.5991400 0.1156350 0.3304760
2.4904900 0.6125950 0.4491460
0.9445400 0.3937990 0.2657040
0 1 3 3 1
1.2779000 -0.2276060 -0.0175130
0.3975900 0.00144583 0.2445330
0.1600950 1.0927900 0.8049340
0 1 1 0 1
0.1 1. 1.
0 3 1 0 1
0.325 1.0
15 12
0 0 6 2 1
77492.4000000 0.0007810
11605.8000000 0.0060680
2645.9600000 0.0311600
754.9760000 0.1234310
248.7550000 0.3782090

91.1565000 0.5632620
0 0 3 2 1
91.1565000 0.1602550
36.2257000 0.6276470
15.2113000 0.2638490
0 0 1 2 1
4.7941700 1.0000000
0 0 1 0 1
1.8079300 1.0000000
0 0 1 0 1
0.3568160 1.0000000
0 0 1 0 1
0.1147830 1.0000000
0 2 4 6 1
384.8430000 0.0092060
90.5521000 0.0698740
29.1339000 0.2924700
10.8862000 0.7281030
0 2 2 3 1
4.3525900 0.6283490
1.7770600 0.4280440
0 2 1 0 1
0.6970050 1.0000000
0 2 1 0 1
0.2535320 1.0000000
0 2 1 0 1
0.1 1.0000000
0 3 1 0 1
0.5500000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE

30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

CdS

CdS – Journal of Magnetism and Magnetic Materials (1996) 152, p159-p164
crystal
0 0 0
216
5.8304
2
248 0 0 0
16 0.25 0.25 0.25
printout
basisset
end
end
248 10
input
20. 0 2 4 4 2 0
13.355176 270.039448 0
7.308378 38.877766 0
12.659728 64.607470 0
12.289639 129.219445 0
6.786176 10.622558 0
6.400743 21.265046 0
11.161722 31.663965 0
11.219615 47.489216 0
4.537733 5.186200 0
4.335727 7.566063 0
11.478986 -12.632785 0
11.487027 -16.760171 0
0 0 7 2 1
0.22385300e+03 0.87100000e-03
0.23094800e+02 -0.64307000e-01
0.14652200e+02 0.30131600e+00
0.65704440e+01 -0.76052400e+00
0.15378300e+01 0.89407100e+00
0.69098400e+00 0.42787900e+00
0.13491300e+00 0.10188000e-01
0 0 7 2 1
0.22385300e+03 -0.22900000e-03
0.23094800e+02 0.15594000e-01
0.14652200e+02 -0.81047000e-01
0.65704440e+01 0.22725100e+00
0.15378300e+01 -0.36256300e+00
0.69098400e+00 -0.25078300e+00
0.13491300e+00 0.61353300e+00

0 0 7 0 1
0.22385300e+03 0.10770000e-02
0.23094800e+02 -0.71649000e-01
0.14652200e+02 0.28897500e+00
0.65704440e+01 -0.73154600e+00
0.15378300e+01 0.19768990e+01
0.69098400e+00 -0.13519510e+01
0.13491300e+00 -0.11186740e+01
0 0 1 0 1
0.07 0.10000000e+01
0 2 6 6 1
0.13717500e+02 0.77616000e-01
0.84632200e+01 -0.25794300e+00
0.21182000e+01 0.53527400e+00
0.98926200e+00 0.49636200e+00
0.43178100e+00 0.12310900e+00
0.13916000e+00 0.32100000e-02
0 2 6 0 1
0.13717500e+02 -0.30730000e-01
0.84632200e+01 0.10874400e+00
0.21182000e+01 -0.27823100e+00
0.98926200e+00 -0.32939000e+00
0.43178100e+00 0.35463000e+00
0.13916000e+00 0.78145800e+00
0 2 1 0 1
0.09 0.10000000e+01
0 3 6 10 1
0.31669700e+02 0.31630000e-02
0.12221400e+02 -0.11791000e-01
0.31219900e+01 0.24119400e+00
0.13894100e+01 0.44899800e+00
0.57320300e+00 0.38021100e+00
0.21170800e+00 0.14455300e+00
0 3 6 0 1
0.31669700e+02 -0.48710000e-02
0.12221400e+02 0.18582000e-01
0.31219900e+01 -0.47667300e+00
0.13894100e+01 -0.45760400e+00
0.57320300e+00 0.57146200e+00
0.21170800e+00 0.49738000e+00
0 3 1 0 1
0.21170800e+00 0.10000000e+01
16 12
0 0 6 2 1
93413.4000000 0.0007430

13961.7000000 0.0057930
3169.9100000 0.0299540
902.4560000 0.1190280
297.1580000 0.3684320
108.7020000 0.5772990
0 0 3 2 1
108.7020000 0.1431860
43.1553000 0.6244650
18.1079000 0.2833660
0 0 1 2 1
5.5600900 1.0000000
0 0 1 0 1
2.1318300 1.0000000
0 0 1 0 1
0.4204030 1.0000000
0 0 1 0 1
0.1360450 1.0000000
0 2 4 6 1
495.0400000 0.0083090
117.2210000 0.0640240
37.7749000 0.2776140
14.0584000 0.7450760
0 2 2 4 1
5.5657400 0.6137120
2.2629700 0.4438180
0 2 1 0 1
0.8079940 1.0000000
0 2 1 0 1
0.2774600 1.0000000
0 2 1 0 1
0.1 1.
0 3 1 0 1
0.6500000 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
10 0 20

maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

AgBr

AgBr – Physical Review, Serie 3. B - Condensed Matter (18,1978-) (1999) 59, p750-p761
crystal
0 0 0
225
5.7721
2
247 0.00 0.00 0.00
235 0.5 0.5 0.5
printout
basisset
end
end
247 11
input
19. 0 2 4 4 2 0
12.567714 255.054771 0
6.997662 36.983393 0
11.316496 60.715705 0
10.958063 121.443889 0
7.111400 10.171866 0
6.773319 20.486564 0
8.928437 29.504938 0
11.102567 44.018736 0
5.543212 5.368333 0
3.928835 7.408375 0
11.012913 -12.623403 0
11.019898 -16.764327 0
0 0 7 2 1
0.18007500E+03 0.84900000E-03
0.21898700E+02 -0.65450000E-01
0.13867000E+02 0.29776500E+00
0.61426300E+01 -0.75312100E+00
0.14381400E+01 0.88117500E+00
0.64838200E+00 0.43517600E+00
0.12888200E+00 0.14738000E-01
0 0 7 2 1
0.18007500E+03 -0.20300000E-03
0.21898700E+02 0.15723000E-01
0.13867000E+02 -0.79229000E-01
0.61426300E+01 0.22263400E+00
0.14381400E+01 -0.34919600E+00
0.64838200E+00 -0.25597800E+00
0.12888200E+00 0.54866600E+00

0 0 7 0 1
0.18007500E+03 -0.86200000E-03
0.21898700E+02 0.52546000E-01
0.13867000E+02 -0.20810000E+00
0.61426300E+01 0.52497200E+00
0.14381400E+01 -0.12701730E+01
0.64838200E+00 0.53937300E+00
0.12888200E+00 0.16533910E+01
0 0 1 0 1
0.12 0.10000000E+01
0 2 6 6 1
0.11875100E+02 0.11624800E+00
0.80024500E+01 -0.30728600E+00
0.20176600E+01 0.51573600E+00
0.95423000E+00 0.50310400E+00
0.42311800E+00 0.14209500E+00
0.13588500E+00 0.51530000E-02
0 2 6 0 1
0.11875100E+02 -0.28284000E-01
0.80024500E+01 0.78347000E-01
0.20176600E+01 -0.15674100E+00
0.95423000E+00 -0.18862500E+00
0.42311800E+00 0.63565000E-01
0.13588500E+00 0.58177800E+00
0 2 6 0 1
0.11875100E+02 -0.52857000E-01
0.80024500E+01 0.14703900E+00
0.20176600E+01 -0.31297300E+00
0.95423000E+00 -0.37082800E+00
0.42311800E+00 0.42362900E+00
0.13588500E+00 0.75365500E+00
0 2 1 0 1
0.12 0.10000000E+01
0 3 6 9 1
0.26432000E+02 0.34790000E-02
0.11034500E+02 -0.13848000E-01
0.27378700E+01 0.25459900E+00
0.11957500E+01 0.44984900E+00
0.48204200E+00 0.37573800E+00
0.17290800E+00 0.14587900E+00
0 3 6 0 1
0.26432000E+02 -0.47330000E-02
0.11034500E+02 0.19070000E-01
0.27378700E+01 -0.43329800E+00
0.11957500E+01 -0.44456800E+00

0.48204200E+00 0.49144200E+00
0.17290800E+00 0.57286600E+00
0 3 1 0 1
0.17290800E+00 0.10000000E+01
235 9
input
25. 0 3 4 6 2 0
70.024257 49.962834 0
31.178412 370.014205 0
7.156593 10.241439 0
46.773471 99.112244 0
46.184120 198.253046 0
21.713858 28.261740 0
20.941792 56.623366 0
50.698839 -18.605853 0
50.644764 -27.923280 0
15.447509 -0.379693 0
15.500259 -0.780583 0
2.800391 0.035968 0
1.077480 0.094397 0
14.465606 -1.091269 0
21.234065 -2.887691 0
0 0 8 2 1
2808.60 0.001606
421.180 0.008393
50.3457 0.069578
17.9133 -0.389908
3.80531 0.694497
1.74968 0.491354
0.448555 0.022637
0.164498 -0.003723
0 0 8 2 1
2808.60 -0.000635
421.180 -0.003492
50.3457 -0.025195
17.9133 0.150113
3.80531 -0.366226
1.74968 -0.383422
0.448555 0.714468
0.164498 0.535253
0 0 1 0 1
0.448555 1
0 0 1 0 1
0.164498 1
0 2 7 6 1

105.752 0.005341
27.6368 -0.083084
6.59656 0.447766
2.78522 0.550617
1.07812 0.123500
0.393537 -0.003771
0.127469 0.002278
0 2 7 5 1
105.752 -0.001308
27.6368 0.022921
6.59656 -0.145029
2.78522 -0.209037
1.07812 0.093730
0.393537 0.605021
0.127469 0.457123
0 2 1 0 1
0.127469 1
0 3 6 10 1
143.865 0.010237
46.1163 0.076083
17.3694 0.229807
6.95107 0.403347
2.75607 0.409728
1.01178 0.162790
0 3 1 0 1
0.4291 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
sorestart
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80

broyden
0.0001
end

ZnSe

ZnSe – Kristallografiya (1997) 42, p649-p659
crystal
0 0 0
216
5.6740
2
230 0.000 0.000 0.000
234 0.25 0.25 0.25
printout
basisset
end
end
230 10
input
20. 0 2 4 4 2 0
34.174001 399.986399 0
14.456371 85.489750 0
39.888683 92.381077 0
39.655017 184.771176 0
15.290546 23.002541 0
14.903524 46.057427 0
43.708296 -13.690734 0
43.698536 -20.543980 0
15.150718 -1.316154 0
15.282441 -1.838715 0
8.160014 -0.370360 0
12.228422 -1.062943 0
0 0 7 2 1
0.62912600e+03 0.55900000e-03
0.62963500e+02 -0.96800000e-02
0.39579100e+02 0.62354000e-01
0.11917300e+02 -0.41487900e+00
0.25082400e+01 0.75446600e+00
0.10301900e+01 0.45899600e+00
0.15400200e+00 0.11664000e-01
0 0 7 2 1
0.62912600e+03 -0.12100000e-03
0.62963500e+02 0.14890000e-02
0.39579100e+02 -0.12737000e-01
0.11917300e+02 0.97246000e-01
0.25082400e+01 -0.21991700e+00
0.10301900e+01 -0.23647400e+00
0.15400200e+00 0.58129100e+00

0 0 7 0 1
0.62912600e+03 0.42100000e-03
0.62963500e+02 -0.51090000e-02
0.39579100e+02 0.41447000e-01
0.11917300e+02 -0.34164300e+00
0.25082400e+01 0.14386170e+01
0.10301900e+01 -0.98242900e+00
0.15400200e+00 -0.11876310e+01
0 0 1 0 1
0.1 0.10000000e+01
0 2 6 6 1
0.92903400e+02 0.24880000e-02
0.19745200e+02 -0.79136000e-01
0.45507300e+01 0.38805900e+00
0.20019000e+01 0.50935400e+00
0.84387900e+00 0.22457500e+00
0.20338100e+00 0.12680000e-01
0 2 6 0 1
0.92903400e+02 -0.53000000e-03
0.19745200e+02 0.24743000e-01
0.45507300e+01 -0.14247800e+00
0.20019000e+01 -0.23403200e+00
0.84387900e+00 0.92187000e-01
0.20338100e+00 0.83777000e+00
0 2 1 0 1
0.59572000e-01 0.10000000e+01
0 3 6 10 1
0.71276600e+02 0.15895000e-01
0.22760400e+02 0.92454000e-01
0.83236900e+01 0.25947200e+00
0.31687500e+01 0.40331400e+00
0.11470300e+01 0.38783400e+00
0.36664300e+00 0.20225800e+00
0 3 6 0 1
0.71276600e+02 -0.22516000e-01
0.22760400e+02 -0.13330300e+00
0.83236900e+01 -0.39325300e+00
0.31687500e+01 -0.35121400e+00
0.11470300e+01 0.40617100e+00
0.36664300e+00 0.57920500e+00
0 3 1 0 1
0.36664300e+00 0.10000000e+01
234 9
input
24. 0 2 4 6 2 0

30.046990 370.122888 0
6.918688 10.456168 0
45.773014 99.135059 0
45.294642 198.292483 0
20.739648 28.338747 0
20.028601 56.749747 0
50.941768 -18.526556 0
49.594740 -28.334921 0
16.323522 -0.696089 0
14.465196 -1.167891 0
3.775330 0.041443 0
3.501953 0.235583 0
11.950867 -0.766262 0
17.810780 -2.102742 0
0 0 8 2.0 1
2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.021091
0.1399 -0.003916
0 0 8 2.0 1
2609.7204 -0.000694
391.5228 -0.003866
48.2893 -0.024839
16.8019 0.140207
3.5149 -0.342280
1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
0 0 1 0. 1
0.3830 1
0 0 1 0. 1
0.1399 1
0 2 7 6.0 1
100.0192 0.004761
25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
0 2 7 4.0 1

100.0192 -0.001058
25.8909 0.021709
6.2093 -0.126243
2.6613 -0.193545
1.0929 0.047373
0.3597 0.591806
0.1137 0.499759
0 2 1 0. 1
0.1137 1
0 3 6 10. 1
128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0 3 1 0. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.001
end

AgI

AgI – Physical Review, Serie 3. B - Condensed Matter (18,1978-) (1999) 59, p750-p761
crystal
0 0 0
216
6.4991
2
247 0.25 0.25 0.25
253 0.00 0.00 0.00
printout
basisset
end
end
247 11
input
19. 0 2 4 4 2 0
12.567714 255.054771 0
6.997662 36.983393 0
11.316496 60.715705 0
10.958063 121.443889 0
7.111400 10.171866 0
6.773319 20.486564 0
8.928437 29.504938 0
11.102567 44.018736 0
5.543212 5.368333 0
3.928835 7.408375 0
11.012913 -12.623403 0
11.019898 -16.764327 0
0 0 7 2 1
0.18007500E+03 0.84900000E-03
0.21898700E+02 -0.65450000E-01
0.13867000E+02 0.29776500E+00
0.61426300E+01 -0.75312100E+00
0.14381400E+01 0.88117500E+00
0.64838200E+00 0.43517600E+00
0.12888200E+00 0.14738000E-01
0 0 7 2 1
0.18007500E+03 -0.20300000E-03
0.21898700E+02 0.15723000E-01
0.13867000E+02 -0.79229000E-01
0.61426300E+01 0.22263400E+00
0.14381400E+01 -0.34919600E+00
0.64838200E+00 -0.25597800E+00
0.12888200E+00 0.54866600E+00

0 0 7 0 1
0.18007500E+03 -0.86200000E-03
0.21898700E+02 0.52546000E-01
0.13867000E+02 -0.20810000E+00
0.61426300E+01 0.52497200E+00
0.14381400E+01 -0.12701730E+01
0.64838200E+00 0.53937300E+00
0.12888200E+00 0.16533910E+01
0 0 1 0 1
0.12 0.10000000E+01
0 2 6 6 1
0.11875100E+02 0.11624800E+00
0.80024500E+01 -0.30728600E+00
0.20176600E+01 0.51573600E+00
0.95423000E+00 0.50310400E+00
0.42311800E+00 0.14209500E+00
0.13588500E+00 0.51530000E-02
0 2 6 0 1
0.11875100E+02 -0.28284000E-01
0.80024500E+01 0.78347000E-01
0.20176600E+01 -0.15674100E+00
0.95423000E+00 -0.18862500E+00
0.42311800E+00 0.63565000E-01
0.13588500E+00 0.58177800E+00
0 2 6 0 1
0.11875100E+02 -0.52857000E-01
0.80024500E+01 0.14703900E+00
0.20176600E+01 -0.31297300E+00
0.95423000E+00 -0.37082800E+00
0.42311800E+00 0.42362900E+00
0.13588500E+00 0.75365500E+00
0 2 1 0 1
0.12 0.10000000E+01
0 3 6 9 1
0.26432000E+02 0.34790000E-02
0.11034500E+02 -0.13848000E-01
0.27378700E+01 0.25459900E+00
0.11957500E+01 0.44984900E+00
0.48204200E+00 0.37573800E+00
0.17290800E+00 0.14587900E+00
0 3 6 0 1
0.26432000E+02 -0.47330000E-02
0.11034500E+02 0.19070000E-01
0.27378700E+01 -0.43329800E+00
0.11957500E+01 -0.44456800E+00

0.48204200E+00 0.49144200E+00
0.17290800E+00 0.57286600E+00
0 3 1 0 1
0.17290800E+00 0.10000000E+01
253 9
input
25. 0 3 4 4 4 0
40.033376 49.989649 0
17.300576 281.006556 0
8.851720 61.416739 0
15.720141 67.416239 0
15.208222 134.807696 0
8.294186 14.566548 0
7.753949 28.968422 0
13.817751 35.538756 0
13.587805 53.339759 0
6.947630 9.716466 0
6.960099 14.977500 0
18.522950 -20.176618 0
18.251035 -26.088077 0
7.557901 -0.220434 0
7.597404 -0.221646 0
0 0 8 2 1
0.24497900e+04 0.41900000e-03
0.35980800e+03 0.22400000e-02
0.14405800e+02 0.39722300e+00
0.90763200e+01 -0.93224900e+00
0.20881000e+01 0.93713800e+00
0.10349800e+01 0.39208600e+00
0.31628400e+00 0.12485000e-01
0.12171900e+00 -0.13290000e-02
0 0 8 2 1
0.24497900e+04 0.17500000e-03
0.35980800e+03 0.10570000e-02
0.14405800e+02 0.16900000e+00
0.90763200e+01 -0.42179300e+00
0.20881000e+01 0.63886400e+00
0.10349800e+01 0.32011500e+00
0.31628400e+00 -0.81442800e+00
0.12171900e+00 -0.48979800e+00
0 0 1 0 1
0.31628400e+00 0.10000000e+01
0 0 1 0 1
0.12171900e+00 0.10000000e+01
0 2 6 6 1

0.19530100e+02 0.58934000e-01
0.11088200e+02 -0.23093000e+00
0.27156300e+01 0.66480100e+00
0.12043000e+01 0.45067300e+00
0.33994500e+00 0.28980000e-01
0.11088100e+00 -0.28890000e-02
0 2 6 5 1
0.19530100e+02 -0.18836000e-01
0.11088200e+02 0.80006000e-01
0.27156300e+01 -0.30665200e+00
0.12043000e+01 -0.14759400e+00
0.33994500e+00 0.60750600e+00
0.11088100e+00 0.54704900e+00
0 2 1 0 1
0.11088100e+00 0.10000000e+01
0 3 6 10 1
0.45476500e+02 0.42660000e-02
0.13192800e+02 -0.13625000e-01
0.42274100e+01 0.30975600e+00
0.19428000e+01 0.50977200e+00
0.83977100e+00 0.29746100e+00
0.30000000e+00 0.40164000e-01
0 3 1 0 1
0.30000000e+00 0.10000000e+01
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

SiC (6H)

SiC (6H)– American Mineralogist (2007) 92, p403-p407
CRYSTAL
0 0 0
186
3.0810 15.1248
6
14 0.0 0.0 0.0
14 0.33333333 0.6666667 0.3336
14 0.33333333 0.6666667 0.6671
6 0.33333333 0.6666667 0.4588
6 0.0 0.0 0.1254
6 0.33333333 0.6666667 0.7920
PRINTOUT
BASISSET
END
END
14 5
0 0 6 2 1
16115.9000000 0.00195948
2425.5800000 0.01492880
553.8670000 0.07284780
156.3400000 0.24613000
50.0683000 0.48591400
17.0178000 0.32500200
0 1 6 8 1
292.7180000 -0.00278094 0.00443826
69.8731000 -0.03571460 0.03266790
22.3363000 -0.11498500 0.13472100
8.1503900 0.09356340 0.32867800
3.1345800 0.60301700 0.44964000
1.2254300 0.41895900 0.26137200
0 1 3 4 1
1.7273800 -0.24463000 -0.01779510
0.5729220 0.00431572 0.25353900
0.2221920 1.09818000 0.80066900
0 1 1 0 1
0.12 1.00000000 1.00000000
0 3 1 0 1
0.4500000 1.0000000
6 5
0 0 6 2 1
4563.2400000 0.00196665
682.0240000 0.0152306

154.9730000 0.0761269
44.4553000 0.2608010
13.0290000 0.6164620
1.8277300 0.2210060
0 1 3 4 1
20.9642000 0.1146600 0.0402487
4.8033100 0.9199990 0.2375940
1.4593300 -0.00303068 0.8158540
0 1 1 0 1
0.4834560 1.0000000 1.0000000
0 1 1 0 1
0.1455850 1.0000000 1.0000000
0 3 1 0 1
0.6260000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
20
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

CuBr

CuBr – Journal of the American Chemical Society (1922) 44, p30-p36
crystal
0 0 0
216
5.82
2
229 0.00 0.00 0.00
235 0.25 0.25 0.25
printout
basisset
end
end
229 10
input
19. 0 2 4 4 2 0
30.110543 355.750512 0
13.076310 70.930906 0
32.692614 77.969931 0
32.770339 155.927448 0
13.751067 18.021132 0
13.322166 36.094372 0
38.996511 -12.343410 0
39.539788 -18.273362 0
12.287511 -0.984705 0
11.459300 -1.318747 0
6.190102 -0.227264 0
8.118780 -0.468773 0
0 0 7 2 1
0.56008800e+03 0.63700000e-03
0.56648600e+02 -0.97350000e-02
0.35425800e+02 0.65793000e-01
0.11054600e+02 -0.41503500e+00
0.23068200e+01 0.74661100e+00
0.95142900e+00 0.46217300e+00
0.14518400e+00 0.15983000e-01
0 0 7 1 1
0.56008800e+03 -0.13600000e-03
0.56648600e+02 0.14010000e-02
0.35425800e+02 -0.13174000e-01
0.11054600e+02 0.95695000e-01
0.23068200e+01 -0.21187400e+00
0.95142900e+00 -0.23594400e+00
0.14518400e+00 0.50811500e+00

0 0 7 0 1
0.56008800e+03 -0.33300000e-03
0.56648600e+02 0.59300000e-02
0.35425800e+02 -0.32549000e-01
0.11054600e+02 0.21107100e+00
0.23068200e+01 -0.73055600e+00
0.95142900e+00 0.17724200e+00
0.14518400e+00 0.17148730e+01
0 0 1 0 1
0.12 0.10000000e+01
0 2 6 6 1
0.70973900e+02 0.36820000e-02
0.17851000e+02 -0.82128000e-01
0.42467900e+01 0.37537900e+00
0.18776000e+01 0.50840900e+00
0.79333500e+00 0.23909500e+00
0.19347600e+00 0.15850000e-01
0 2 6 0 1
0.70973900e+02 -0.62800000e-03
0.17851000e+02 0.16563000e-01
0.42467900e+01 -0.84572000e-01
0.18776000e+01 -0.14128300e+00
0.79333500e+00 -0.35710000e-02
0.19347600e+00 0.51900500e+00
0 2 1 0 1
0.12 0.10000000e+01
0 3 6 10 1
0.60380400e+02 0.17564000e-01
0.19112100e+02 0.99134000e-01
0.69528800e+01 0.27117100e+00
0.26099400e+01 0.40618000e+00
0.92256700e+00 0.38142700e+00
0.28364200e+00 0.20062600e+00
0 3 6 0 1
0.60380400e+02 -0.22286000e-01
0.19112100e+02 -0.12827400e+00
0.69528800e+01 -0.36279700e+00
0.26099400e+01 -0.32572200e+00
0.92256700e+00 0.32708700e+00
0.28364200e+00 0.65680900e+00
0 3 1 0 1
0.28364200e+00 0.10000000e+01
235 9
input
25. 0 3 4 6 2 0

70.024257 49.962834 0
31.178412 370.014205 0
7.156593 10.241439 0
46.773471 99.112244 0
46.184120 198.253046 0
21.713858 28.261740 0
20.941792 56.623366 0
50.698839 -18.605853 0
50.644764 -27.923280 0
15.447509 -0.379693 0
15.500259 -0.780583 0
2.800391 0.035968 0
1.077480 0.094397 0
14.465606 -1.091269 0
21.234065 -2.887691 0
0 0 8 2 1
2808.60 0.001606
421.180 0.008393
50.3457 0.069578
17.9133 -0.389908
3.80531 0.694497
1.74968 0.491354
0.448555 0.022637
0.164498 -0.003723
0 0 8 2 1
2808.60 -0.000635
421.180 -0.003492
50.3457 -0.025195
17.9133 0.150113
3.80531 -0.366226
1.74968 -0.383422
0.448555 0.714468
0.164498 0.535253
0 0 1 0 1
0.448555 1
0 0 1 0 1
0.164498 1
0 2 7 6 1
105.752 0.005341
27.6368 -0.083084
6.59656 0.447766
2.78522 0.550617
1.07812 0.123500
0.393537 -0.003771
0.127469 0.002278

0 2 7 5 1
105.752 -0.001308
27.6368 0.022921
6.59656 -0.145029
2.78522 -0.209037
1.07812 0.093730
0.393537 0.605021
0.127469 0.457123
0 2 1 0 1
0.127469 1
0 3 6 10 1
143.865 0.010237
46.1163 0.076083
17.3694 0.229807
6.95107 0.403347
2.75607 0.409728
1.01178 0.162790
0 3 1 0 1
0.4291 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

CuI

CuI – Canadian Mineralogist (1997) 35, p785-p786
crystal
0 0 0
216
6.063
2
229 0.25 0.25 0.25
253 0.00 0.00 0.00
printout
basisset
end
end
229 10
input
19. 0 2 4 4 2 0
30.110543 355.750512 0
13.076310 70.930906 0
32.692614 77.969931 0
32.770339 155.927448 0
13.751067 18.021132 0
13.322166 36.094372 0
38.996511 -12.343410 0
39.539788 -18.273362 0
12.287511 -0.984705 0
11.459300 -1.318747 0
6.190102 -0.227264 0
8.118780 -0.468773 0
0 0 7 2 1
0.56008800e+03 0.63700000e-03
0.56648600e+02 -0.97350000e-02
0.35425800e+02 0.65793000e-01
0.11054600e+02 -0.41503500e+00
0.23068200e+01 0.74661100e+00
0.95142900e+00 0.46217300e+00
0.14518400e+00 0.15983000e-01
0 0 7 1 1
0.56008800e+03 -0.13600000e-03
0.56648600e+02 0.14010000e-02
0.35425800e+02 -0.13174000e-01
0.11054600e+02 0.95695000e-01
0.23068200e+01 -0.21187400e+00
0.95142900e+00 -0.23594400e+00
0.14518400e+00 0.50811500e+00

0 0 7 0 1
0.56008800e+03 -0.33300000e-03
0.56648600e+02 0.59300000e-02
0.35425800e+02 -0.32549000e-01
0.11054600e+02 0.21107100e+00
0.23068200e+01 -0.73055600e+00
0.95142900e+00 0.17724200e+00
0.14518400e+00 0.17148730e+01
0 0 1 0 1
0.12 0.10000000e+01
0 2 6 6 1
0.70973900e+02 0.36820000e-02
0.17851000e+02 -0.82128000e-01
0.42467900e+01 0.37537900e+00
0.18776000e+01 0.50840900e+00
0.79333500e+00 0.23909500e+00
0.19347600e+00 0.15850000e-01
0 2 6 0 1
0.70973900e+02 -0.62800000e-03
0.17851000e+02 0.16563000e-01
0.42467900e+01 -0.84572000e-01
0.18776000e+01 -0.14128300e+00
0.79333500e+00 -0.35710000e-02
0.19347600e+00 0.51900500e+00
0 2 1 0 1
0.12 0.10000000e+01
0 3 6 10 1
0.60380400e+02 0.17564000e-01
0.19112100e+02 0.99134000e-01
0.69528800e+01 0.27117100e+00
0.26099400e+01 0.40618000e+00
0.92256700e+00 0.38142700e+00
0.28364200e+00 0.20062600e+00
0 3 6 0 1
0.60380400e+02 -0.22286000e-01
0.19112100e+02 -0.12827400e+00
0.69528800e+01 -0.36279700e+00
0.26099400e+01 -0.32572200e+00
0.92256700e+00 0.32708700e+00
0.28364200e+00 0.65680900e+00
0 3 1 0 1
0.28364200e+00 0.10000000e+01
253 9
input
25. 0 3 4 4 4 0

40.033376 49.989649 0
17.300576 281.006556 0
8.851720 61.416739 0
15.720141 67.416239 0
15.208222 134.807696 0
8.294186 14.566548 0
7.753949 28.968422 0
13.817751 35.538756 0
13.587805 53.339759 0
6.947630 9.716466 0
6.960099 14.977500 0
18.522950 -20.176618 0
18.251035 -26.088077 0
7.557901 -0.220434 0
7.597404 -0.221646 0
0 0 8 2 1
0.24497900e+04 0.41900000e-03
0.35980800e+03 0.22400000e-02
0.14405800e+02 0.39722300e+00
0.90763200e+01 -0.93224900e+00
0.20881000e+01 0.93713800e+00
0.10349800e+01 0.39208600e+00
0.31628400e+00 0.12485000e-01
0.12171900e+00 -0.13290000e-02
0 0 8 2 1
0.24497900e+04 0.17500000e-03
0.35980800e+03 0.10570000e-02
0.14405800e+02 0.16900000e+00
0.90763200e+01 -0.42179300e+00
0.20881000e+01 0.63886400e+00
0.10349800e+01 0.32011500e+00
0.31628400e+00 -0.81442800e+00
0.12171900e+00 -0.48979800e+00
0 0 1 0 1
0.31628400e+00 0.10000000e+01
0 0 1 0 1
0.12171900e+00 0.10000000e+01
0 2 6 6 1
0.19530100e+02 0.58934000e-01
0.11088200e+02 -0.23093000e+00
0.27156300e+01 0.66480100e+00
0.12043000e+01 0.45067300e+00
0.33994500e+00 0.28980000e-01
0.11088100e+00 -0.28890000e-02
0 2 6 5 1

0.19530100e+02 -0.18836000e-01
0.11088200e+02 0.80006000e-01
0.27156300e+01 -0.30665200e+00
0.12043000e+01 -0.14759400e+00
0.33994500e+00 0.60750600e+00
0.11088100e+00 0.54704900e+00
0 2 1 0 1
0.11088100e+00 0.10000000e+01
0 3 6 10 1
0.45476500e+02 0.42660000e-02
0.13192800e+02 -0.13625000e-01
0.42274100e+01 0.30975600e+00
0.19428000e+01 0.50977200e+00
0.83977100e+00 0.29746100e+00
0.30000000e+00 0.40164000e-01
0 3 1 0 1
0.30000000e+00 0.10000000e+01
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

CoO

CoO – Proceedings of the Japan Academy (1979) 55, p43-p48
CRYSTAL
0 0 0
225
4.2630
2
27 0. 0. 0.
8 0.5 0.5 0.5
PRINTOUT
BASISSET
END
SUPERCEL
0. 1. 1. 1. 0. 1. 1. 1. 0.
END
8 4
0 0 6 2 1
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 8 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
27 8
0 0 6 2 1
66148.9900000 1.759787E-03
9933.0770000 1.348162E-02
2262.8160000 6.649342E-02
637.9154000 2.307939E-01
204.4122000 4.792919E-01
69.8253800 3.514097E-01
0 1 6 8 1
1378.8410000 2.376276E-03 3.971488E-03
328.2694000 3.167450E-02 3.108174E-02
106.0946000 1.262888E-01 1.357439E-01
39.8327500 -2.584552E-02 3.476827E-01

16.1862200 -6.183491E-01 4.626340E-01
6.6677880 -4.567008E-01 2.051632E-01
0 1 6 8 1
54.5235500 -3.993004E-03 -7.290772E-03
18.2978300 7.409663E-02 -2.926027E-02
7.8673480 2.542000E-01 6.564150E-02
3.3405340 -2.921657E-01 4.000652E-01
1.3937560 -7.318703E-01 4.950236E-01
0.5513260 -2.040784E-01 1.758240E-01
0 1 3 2 1
2.1519470 0.05379843 -0.2165496
0.8110630 0.2759971 0.1240488
0.1210170 -1.1296920 0.9724064
0 1 1 0 1
0.12 1. 1.
0 3 3 5 1
25.5930600 9.004748E-02
6.8009900 3.931703E-01
2.0516470 6.976844E-01
0 3 1 0 1
0.5556710 1.0000000
0 4 1 0 1
0.8 1.
99 0
END
UHF
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 24
ATOMSPIN
2
1 1 2 -1
SPINLOCK
0 5
SCFDIR
BIPOSIZE
30000000
EXCHSIZE

30000000
MAXCYCLE
100
FMIXING
60
ANDERSON
PPAN
GUESSP
END

AgCl

AgCl – Physical Review, Serie 3. B - Condensed Matter (18,1978-) (1999) 59, p750-p761
crystal
0 0 0
225
5.5463
2
247 0.00 0.00 0.00
17 0.5 0.5 0.5
printout
basisset
end
end
247 11
input
19. 0 2 4 4 2 0
12.567714 255.054771 0
6.997662 36.983393 0
11.316496 60.715705 0
10.958063 121.443889 0
7.111400 10.171866 0
6.773319 20.486564 0
8.928437 29.504938 0
11.102567 44.018736 0
5.543212 5.368333 0
3.928835 7.408375 0
11.012913 -12.623403 0
11.019898 -16.764327 0
0 0 7 2 1
0.18007500E+03 0.84900000E-03
0.21898700E+02 -0.65450000E-01
0.13867000E+02 0.29776500E+00
0.61426300E+01 -0.75312100E+00
0.14381400E+01 0.88117500E+00
0.64838200E+00 0.43517600E+00
0.12888200E+00 0.14738000E-01
0 0 7 2 1
0.18007500E+03 -0.20300000E-03
0.21898700E+02 0.15723000E-01
0.13867000E+02 -0.79229000E-01
0.61426300E+01 0.22263400E+00
0.14381400E+01 -0.34919600E+00
0.64838200E+00 -0.25597800E+00
0.12888200E+00 0.54866600E+00

0 0 7 0 1
0.18007500E+03 -0.86200000E-03
0.21898700E+02 0.52546000E-01
0.13867000E+02 -0.20810000E+00
0.61426300E+01 0.52497200E+00
0.14381400E+01 -0.12701730E+01
0.64838200E+00 0.53937300E+00
0.12888200E+00 0.16533910E+01
0 0 1 0 1
0.12 0.10000000E+01
0 2 6 6 1
0.11875100E+02 0.11624800E+00
0.80024500E+01 -0.30728600E+00
0.20176600E+01 0.51573600E+00
0.95423000E+00 0.50310400E+00
0.42311800E+00 0.14209500E+00
0.13588500E+00 0.51530000E-02
0 2 6 0 1
0.11875100E+02 -0.28284000E-01
0.80024500E+01 0.78347000E-01
0.20176600E+01 -0.15674100E+00
0.95423000E+00 -0.18862500E+00
0.42311800E+00 0.63565000E-01
0.13588500E+00 0.58177800E+00
0 2 6 0 1
0.11875100E+02 -0.52857000E-01
0.80024500E+01 0.14703900E+00
0.20176600E+01 -0.31297300E+00
0.95423000E+00 -0.37082800E+00
0.42311800E+00 0.42362900E+00
0.13588500E+00 0.75365500E+00
0 2 1 0 1
0.12 0.10000000E+01
0 3 6 9 1
0.26432000E+02 0.34790000E-02
0.11034500E+02 -0.13848000E-01
0.27378700E+01 0.25459900E+00
0.11957500E+01 0.44984900E+00
0.48204200E+00 0.37573800E+00
0.17290800E+00 0.14587900E+00
0 3 6 0 1
0.26432000E+02 -0.47330000E-02
0.11034500E+02 0.19070000E-01
0.27378700E+01 -0.43329800E+00
0.11957500E+01 -0.44456800E+00

0.48204200E+00 0.49144200E+00
0.17290800E+00 0.57286600E+00
0 3 1 0 1
0.17290800E+00 0.10000000E+01
17 12
0 0 6 2 1
105819.0000000 0.0007380
15872.0000000 0.0057180
3619.6500000 0.0294950
1030.8000000 0.1172860
339.9080000 0.3629490
124.5380000 0.5841490
0 0 3 2 1
124.5380000 0.1341770
49.5135000 0.6242500
20.8056000 0.2917560
0 0 1 2 1
6.5834600 1.0000000
0 0 1 0 1
2.5646800 1.0000000
0 0 1 0 1
0.5597630 1.0000000
0 0 1 0 1
0.1832730 1.0000000
0 2 5 6 1
589.7760000 0.0023910
139.8490000 0.0185040
45.1413000 0.0813770
16.8733000 0.2215520
6.7411000 0.7725690
0 2 2 5 1
6.7411000 -1.5722440
2.7715200 0.9923890
0 2 1 0 1
1.0238700 1.0000000
0 2 1 0 1
0.3813680 1.0000000
0 2 1 0 1
0.1094370 1.0000000
0 3 1 0 1
0.7500000 1.0000000
99 0
end
uhf
dft

b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
sorestart
end
12 0 24
maxcycle
30
tolscf
7 7
fmixing
80
broyden
0.01
end

SiC (4H)

SiC (4H)– Materials Research Bulletin (1978) 13, (2) p91-p96
CRYSTAL
0 0 0
186
3.0815 10.0614
4
14 0.0 0.0 0.1875
14 0.33333333 0.6666667 0.4375
6 0.0 0.0 0.0
6 0.33333333 0.6666667 0.25
PRINTOUT
BASISSET
END
END
14 5
0 0 6 2 1
16115.9000000 0.00195948
2425.5800000 0.01492880
553.8670000 0.07284780
156.3400000 0.24613000
50.0683000 0.48591400
17.0178000 0.32500200
0 1 6 8 1
292.7180000 -0.00278094 0.00443826
69.8731000 -0.03571460 0.03266790
22.3363000 -0.11498500 0.13472100
8.1503900 0.09356340 0.32867800
3.1345800 0.60301700 0.44964000
1.2254300 0.41895900 0.26137200
0 1 3 4 1
1.7273800 -0.24463000 -0.01779510
0.5729220 0.00431572 0.25353900
0.2221920 1.09818000 0.80066900
0 1 1 0 1
0.12 1.00000000 1.00000000
0 3 1 0 1
0.4500000 1.0000000
6 5
0 0 6 2 1
4563.2400000 0.00196665
682.0240000 0.0152306
154.9730000 0.0761269
44.4553000 0.2608010

13.0290000 0.6164620
1.8277300 0.2210060
0 1 3 4 1
20.9642000 0.1146600 0.0402487
4.8033100 0.9199990 0.2375940
1.4593300 -0.00303068 0.8158540
0 1 1 0 1
0.4834560 1.0000000 1.0000000
0 1 1 0 1
0.1455850 1.0000000 1.0000000
0 3 1 0 1
0.6260000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
20
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

GaN (zincblende)

beta-gan – Madelung
crystal
0 0 0
216
4.531
2
231 0.25 0.25 0.25
7 0. 0. 0.
printout
basisset
end
end
231 9
input
21. 0 2 4 6 2 0
25.880361 370.273040 0
7.901295 9.190615 0
45.149190 99.144001 0
44.979981 198.295512 0
17.224251 28.445653 0
16.747329 56.949705 0
51.968812 -18.168797 0
51.629117 -27.380273 0
15.241738 -1.587022 0
15.320193 -2.516292 0
4.918589 0.083166 0
4.755103 0.202198 0
10.762263 -0.616990 0
19.852939 -3.138584 0
0 0 8 2 1
2848.20 0.000362
420.664 0.002117
29.8118 0.118964
14.2207 -0.461723
2.67643 0.751559
1.13353 0.447202
0.207220 0.012746
0.12 -0.003358
0 0 8 2 1
2848.20 -0.000097
420.664 -0.000614
29.8118 -0.031069
14.2207 0.126784

2.67643 -0.264288
1.13353 -0.275471
0.207220 0.633842
0.12 0.531681
0 0 1 0 1
0.207220 1
0 0 1 0 1
0.12 1
0 2 7 6 1
109.624 0.002101
21.0855 -0.080196
4.92260 0.396415
2.15591 0.519076
0.901913 0.207520
0.202004 0.007825
0.12 -0.001129
0 2 7 1 1
109.624 -0.000288
21.0855 0.013555
4.92260 -0.073629
2.15591 -0.120860
0.901913 -0.001960
0.202004 0.493206
0.12 0.620604
0 2 1 0 1
0.12 1
0 3 7 10 1
85.7978 0.014668
27.6822 0.085621
10.1760 0.248336
3.92208 0.401414
1.45858 0.398604
0.488760 0.186898
0.1772 0.012331
0 3 1 0 1
0.1772 1
7 5
0 0 6 2.0 1.0
6293.4800000 0.00196979
949.0440000 0.0149613
218.7760000 0.0735006
63.6916000 0.2489370
18.8282000 0.6024600
2.7202300 0.2562020
0 1 3 5.0 1.0

30.6331000 0.1119060 0.0383119
7.0261400 0.9216660 0.2374030
2.1120500 -0.00256919 0.8175920
0 1 1 0.0 1.0
0.6840090 1.0000000 1.0000000
0 1 1 0.0 1.0
0.2008780 1.0000000 1.0000000
0 3 1 0.0 1.0
0.9130000 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

SrTiO3

SrTiO3 – Acta Crystallogr Sect B 51 942 (1995)
CRYSTAL
0 0 0
221
3.901
3
238 0.500 0.500 0.5000
222 0 0 0
8 0.5 0 0
PRINTOUT
BASISSET
END
END
238 12
INPUT
10. 0 2 4 4 2 0
6.933460990 135.271042909 0
4.114003832 17.944071402 0
7.216816623 29.438081345 0
7.173696172 58.880674863 0
3.022798817 4.936282692 0
2.865699030 9.723352071 0
6.321514600 11.907239187 0
6.391499495 17.859551440 0
1.769726597 2.199180226 0
1.636771665 2.893570866 0
4.244198396 -5.509333254 0
4.229164471 -7.304641693 0
0 0 7 2 1
328.348319 -0.000056
140.487794 0.000569
63.335426 -0.001642
27.720360 0.006027
12.766925 -0.044662
6.370362 0.332885
3.403661 -0.738465
0 0 1 2 1
1.429397 1.0
0 0 1 0 1
0.471399 1.0
0 0 1 0 1
0.165689 1.0
0 2 4 6 1

49.172539 0.001205
23.366706 -0.005223
10.429117 0.028513
4.892132 -0.097735
0 2 1 0 1
2.129628 1.0
0 2 1 0 1
0.806850 1.0
0 2 1 0 1
0.311271 1.0
0 2 1 0 1
0.127049 1.0
0 3 1 0 1
1.429397 1.0
0 3 1 0 1
0.471399 1.0
0 3 1 0 1
0.165689 1.0
222 10
INPUT
12. 0 2 2 2 0 0
13.010000 158.241593 0
5.862000 17.511824 0
12.460000 95.235127 0
5.217000 10.047856 0
15.350000 -17.568861 0
4.980000 -0.587256 0
0 0 3 2 1
10.7803650 1.7838920
9.7170130 -2.0006890
4.5077550 -0.7563330
0 0 1 2 1
1.2467080 1.0
0 0 1 0 1
0.5087070 1.0
0 0 1 0 1
0.0734380 1.0
0 2 2 6 1
17.5663810 0.0886010
7.7058440 -1.0707460
0 2 2 0 1
3.3291380 0.2001090
1.3081040 0.8379860
0 2 1 0 1
0.4544820 1.0

0 2 1 0 1
0.0717720 1.0
0 3 4 2 1
19.5191940 0.0358140
5.8646130 0.1723730
1.9280380 0.4251360
0.6065630 0.6025950
0 3 1 0 1
0.1639610 1.0
8 4
0 0 6 2.0 1.0
0.5484671660D+04 0.1831074430D-02
0.8252349460D+03 0.1395017220D-01
0.1880469580D+03 0.6844507810D-01
0.5296450000D+02 0.2327143360D+00
0.1689757040D+02 0.4701928980D+00
0.5799635340D+01 0.3585208530D+00
0 1 3 6.0 1.0
0.1553961625D+02 -0.1107775490D+00 0.7087426820D-01
0.3599933586D+01 -0.1480262620D+00 0.3397528390D+00
0.1013761750D+01 0.1130767010D+01 0.7271585770D+00
0 1 1 0.0 1.0
0.2742D+00 0.1000000000D+01 .1000000000D+01
0 3 1 0.0 1.0
0.538D+00 0.1000000000D+01
99 0
END
UHF
DFT
B3PW
END
BIPOSIZE
8000000
EXCHSIZE
8000000
SHRINK
10 20
TOLINTEG
7 7 7 7 14
MAXCYCLE
30
FMIXING
60
ANDERSON
PPAN

END

TiO_2 (Rutile)

```
Rutile TiO2 (295K) – JACS 109 3639 (1987)
CRYSTAL
0 0 0
136
4.59308 2.95889
2
222 0.000 0.0 0.0
8 0.3048 0.3048 0.0
PRINTOUT
BASISSET
END
END
222 10
INPUT
12.  0 2 2 2 0 0
13.010000 158.241593 0
5.862000 17.511824 0
12.460000 95.235127 0
5.217000 10.047856 0
15.350000 -17.568861 0
4.980000 -0.587256 0
0 0 3 2 1
10.7803650 1.7838920
9.7170130 -2.0006890
4.5077550 -0.7563330
0 0 1 2 1
1.2467080 1.0
0 0 1 0 1
0.5087070 1.0
0 0 1 0 1
0.0734380 1.0
0 2 2 6 1
17.5663810 0.0886010
7.7058440 -1.0707460
0 2 2 0 1
3.3291380 0.2001090
1.3081040 0.8379860
0 2 1 0 1
0.4544820 1.0
0 2 1 0 1
0.0717720 1.0
0 3 4 2 1
19.5191940 0.0358140
```

5.8646130 0.1723730
1.9280380 0.4251360
0.6065630 0.6025950
0 3 1 0 1
0.1639610 1.0
8 4
0 0 6 2.0 1.0
0.5484671660D+04 0.1831074430D-02
0.8252349460D+03 0.1395017220D-01
0.1880469580D+03 0.6844507810D-01
0.5296450000D+02 0.2327143360D+00
0.1689757040D+02 0.4701928980D+00
0.5799635340D+01 0.3585208530D+00
0 1 3 6.0 1.0
0.1553961625D+02 -0.1107775490D+00 0.7087426820D-01
0.3599933586D+01 -0.1480262620D+00 0.3397528390D+00
0.1013761750D+01 0.1130767010D+01 0.7271585770D+00
0 1 1 0.0 1.0
0.2742D+00 0.1000000000D+01 .1000000000D+01
0 3 1 0.0 1.0
0.538D+00 0.1000000000D+01
99 0
END
UHF
DFT
B3PW
END
BIPOSIZE
8000000
EXCHSIZE
8000000
SHRINK
10 20
TOLINTEG
7 7 7 7 14
MAXCYCLE
30
FMIXING
80
ANDERSON
PPAN
END

SiC (2H)

SiC (2H)– Solid State Communications (1979) 32, p783-p785
CRYSTAL
0 0 0
186
3.0790 5.0530
2
14 0.33333333 0.6666667 0.00000
6 0.33333333 0.6666667 0.3760
PRINTOUT
BASISSET
END
END
14 5
0 0 6 2 1
16115.9000000 0.00195948
2425.5800000 0.01492880
553.8670000 0.07284780
156.3400000 0.24613000
50.0683000 0.48591400
17.0178000 0.32500200
0 1 6 8 1
292.7180000 -0.00278094 0.00443826
69.8731000 -0.03571460 0.03266790
22.3363000 -0.11498500 0.13472100
8.1503900 0.09356340 0.32867800
3.1345800 0.60301700 0.44964000
1.2254300 0.41895900 0.26137200
0 1 3 4 1
1.7273800 -0.24463000 -0.01779510
0.5729220 0.00431572 0.25353900
0.2221920 1.09818000 0.80066900
0 1 1 0 1
0.12 1.00000000 1.00000000
0 3 1 0 1
0.4500000 1.0000000
6 5
0 0 6 2 1
4563.2400000 0.00196665
682.0240000 0.0152306
154.9730000 0.0761269
44.4553000 0.2608010
13.0290000 0.6164620
1.8277300 0.2210060

0 1 3 4 1
20.9642000 0.1146600 0.0402487
4.8033100 0.9199990 0.2375940
1.4593300 -0.00303068 0.8158540
0 1 1 0 1
0.4834560 1.0000000 1.0000000
0 1 1 0 1
0.1455850 1.0000000 1.0000000
0 3 1 0 1
0.6260000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
20
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

CuCl

CuCl – Journal of the American Chemical Society (1922) 44, p30-p36
crystal
0 0 0
216
5.501
2
229 0.00 0.00 0.00
17 0.25 0.25 0.25
printout
basisset
end
end
229 10
input
19. 0 2 4 4 2 0
30.110543 355.750512 0
13.076310 70.930906 0
32.692614 77.969931 0
32.770339 155.927448 0
13.751067 18.021132 0
13.322166 36.094372 0
38.996511 -12.343410 0
39.539788 -18.273362 0
12.287511 -0.984705 0
11.459300 -1.318747 0
6.190102 -0.227264 0
8.118780 -0.468773 0
0 0 7 2 1
0.56008800e+03 0.63700000e-03
0.56648600e+02 -0.97350000e-02
0.35425800e+02 0.65793000e-01
0.11054600e+02 -0.41503500e+00
0.23068200e+01 0.74661100e+00
0.95142900e+00 0.46217300e+00
0.14518400e+00 0.15983000e-01
0 0 7 1 1
0.56008800e+03 -0.13600000e-03
0.56648600e+02 0.14010000e-02
0.35425800e+02 -0.13174000e-01
0.11054600e+02 0.95695000e-01
0.23068200e+01 -0.21187400e+00
0.95142900e+00 -0.23594400e+00
0.14518400e+00 0.50811500e+00

0 0 7 0 1
0.56008800e+03 -0.33300000e-03
0.56648600e+02 0.59300000e-02
0.35425800e+02 -0.32549000e-01
0.11054600e+02 0.21107100e+00
0.23068200e+01 -0.73055600e+00
0.95142900e+00 0.17724200e+00
0.14518400e+00 0.17148730e+01
0 0 1 0 1
0.12 0.10000000e+01
0 2 6 6 1
0.70973900e+02 0.36820000e-02
0.17851000e+02 -0.82128000e-01
0.42467900e+01 0.37537900e+00
0.18776000e+01 0.50840900e+00
0.79333500e+00 0.23909500e+00
0.19347600e+00 0.15850000e-01
0 2 6 0 1
0.70973900e+02 -0.62800000e-03
0.17851000e+02 0.16563000e-01
0.42467900e+01 -0.84572000e-01
0.18776000e+01 -0.14128300e+00
0.79333500e+00 -0.35710000e-02
0.19347600e+00 0.51900500e+00
0 2 1 0 1
0.12 0.10000000e+01
0 3 6 10 1
0.60380400e+02 0.17564000e-01
0.19112100e+02 0.99134000e-01
0.69528800e+01 0.27117100e+00
0.26099400e+01 0.40618000e+00
0.92256700e+00 0.38142700e+00
0.28364200e+00 0.20062600e+00
0 3 6 0 1
0.60380400e+02 -0.22286000e-01
0.19112100e+02 -0.12827400e+00
0.69528800e+01 -0.36279700e+00
0.26099400e+01 -0.32572200e+00
0.92256700e+00 0.32708700e+00
0.28364200e+00 0.65680900e+00
0 3 1 0 1
0.28364200e+00 0.10000000e+01
17 12
0 0 6 2 1
105819.0000000 0.0007380

15872.0000000 0.0057180
3619.6500000 0.0294950
1030.8000000 0.1172860
339.9080000 0.3629490
124.5380000 0.5841490
0 0 3 2 1
124.5380000 0.1341770
49.5135000 0.6242500
20.8056000 0.2917560
0 0 1 2 1
6.5834600 1.0000000
0 0 1 0 1
2.5646800 1.0000000
0 0 1 0 1
0.5597630 1.0000000
0 0 1 0 1
0.1832730 1.0000000
0 2 5 6 1
589.7760000 0.0023910
139.8490000 0.0185040
45.1413000 0.0813770
16.8733000 0.2215520
6.7411000 0.7725690
0 2 2 5 1
6.7411000 -1.5722440
2.7715200 0.9923890
0 2 1 0 1
1.0238700 1.0000000
0 2 1 0 1
0.3813680 1.0000000
0 2 1 0 1
0.1094370 1.0000000
0 3 1 0 1
0.7500000 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end

12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

TiO_2 (Anatase)

```
Anatase TiO2 (295K) – JACS 109 3639 (1987)
CRYSTAL
0 0 0
141
3.78479 9.51237
2
222 0.000 0.250 0.3750
8 0.000 0.250 0.1669
PRINTOUT
BASISSET
END
END
222 10
INPUT
12.  0 2 2 2 0 0
13.010000 158.241593 0
5.862000 17.511824 0
12.460000 95.235127 0
5.217000 10.047856 0
15.350000 -17.568861 0
4.980000 -0.587256 0
0 0 3 2 1
10.7803650 1.7838920
9.7170130 -2.0006890
4.5077550 -0.7563330
0 0 1 2 1
1.2467080 1.0
0 0 1 0 1
0.5087070 1.0
0 0 1 0 1
0.0734380 1.0
0 2 2 6 1
17.5663810 0.0886010
7.7058440 -1.0707460
0 2 2 0 1
3.3291380 0.2001090
1.3081040 0.8379860
0 2 1 0 1
0.4544820 1.0
0 2 1 0 1
0.0717720 1.0
0 3 4 2 1
19.5191940 0.0358140
```

5.8646130 0.1723730
1.9280380 0.4251360
0.6065630 0.6025950
0 3 1 0 1
0.1639610 1.0
8 4
0 0 6 2.0 1.0
0.5484671660D+04 0.1831074430D-02
0.8252349460D+03 0.1395017220D-01
0.1880469580D+03 0.6844507810D-01
0.5296450000D+02 0.2327143360D+00
0.1689757040D+02 0.4701928980D+00
0.5799635340D+01 0.3585208530D+00
0 1 3 6.0 1.0
0.1553961625D+02 -0.1107775490D+00 0.7087426820D-01
0.3599933586D+01 -0.1480262620D+00 0.3397528390D+00
0.1013761750D+01 0.1130767010D+01 0.7271585770D+00
0 1 1 0.0 1.0
0.2742D+00 0.1000000000D+01 .1000000000D+01
0 3 1 0.0 1.0
0.538D+00 0.1000000000D+01
99 0
END
UHF
DFT
B3PW
END
BIPOSIZE
8000000
EXCHSIZE
8000000
SHRINK
10 20
TOLINTEG
7 7 7 7 14
MAXCYCLE
30
FMIXING
60
ANDERSON
PPAN
END

ZnO

ZnO – Acta Crystallographica B (24,1968-38,1982) (1969) 25, p1233-p1236
crystal
0 0 0
186
3.2499 5.2066
2
230 0.33333333 0.66666667 0.0000
8 0.33333333 0.66666667 0.6800
printout
basisset
end
end
230 10
input
20. 0 2 4 4 2 0
34.174001 399.986399 0
14.456371 85.489750 0
39.888683 92.381077 0
39.655017 184.771176 0
15.290546 23.002541 0
14.903524 46.057427 0
43.708296 -13.690734 0
43.698536 -20.543980 0
15.150718 -1.316154 0
15.282441 -1.838715 0
8.160014 -0.370360 0
12.228422 -1.062943 0
0 0 7 2 1
0.62912600e+03 0.55900000e-03
0.62963500e+02 -0.96800000e-02
0.39579100e+02 0.62354000e-01
0.11917300e+02 -0.41487900e+00
0.25082400e+01 0.75446600e+00
0.10301900e+01 0.45899600e+00
0.15400200e+00 0.11664000e-01
0 0 7 2 1
0.62912600e+03 -0.12100000e-03
0.62963500e+02 0.14890000e-02
0.39579100e+02 -0.12737000e-01
0.11917300e+02 0.97246000e-01
0.25082400e+01 -0.21991700e+00
0.10301900e+01 -0.23647400e+00
0.15400200e+00 0.58129100e+00

0 0 7 0 1
0.62912600e+03 0.42100000e-03
0.62963500e+02 -0.51090000e-02
0.39579100e+02 0.41447000e-01
0.11917300e+02 -0.34164300e+00
0.25082400e+01 0.14386170e+01
0.10301900e+01 -0.98242900e+00
0.15400200e+00 -0.11876310e+01
0 0 1 0 1
0.1 0.10000000e+01
0 2 6 6 1
0.92903400e+02 0.24880000e-02
0.19745200e+02 -0.79136000e-01
0.45507300e+01 0.38805900e+00
0.20019000e+01 0.50935400e+00
0.84387900e+00 0.22457500e+00
0.20338100e+00 0.12680000e-01
0 2 6 0 1
0.92903400e+02 -0.53000000e-03
0.19745200e+02 0.24743000e-01
0.45507300e+01 -0.14247800e+00
0.20019000e+01 -0.23403200e+00
0.84387900e+00 0.92187000e-01
0.20338100e+00 0.83777000e+00
0 2 1 0 1
0.59572000e-01 0.10000000e+01
0 3 6 10 1
0.71276600e+02 0.15895000e-01
0.22760400e+02 0.92454000e-01
0.83236900e+01 0.25947200e+00
0.31687500e+01 0.40331400e+00
0.11470300e+01 0.38783400e+00
0.36664300e+00 0.20225800e+00
0 3 6 0 1
0.71276600e+02 -0.22516000e-01
0.22760400e+02 -0.13330300e+00
0.83236900e+01 -0.39325300e+00
0.31687500e+01 -0.35121400e+00
0.11470300e+01 0.40617100e+00
0.36664300e+00 0.57920500e+00
0 3 1 0 1
0.36664300e+00 0.10000000e+01
8 4
0 0 6 2 1
5484.6717000 0.0018311

825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 6 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
sorestart
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
6 6
fmixing
80
broyden
0.0001
end

GaN

GaN – Solid State Communications (1977) 23, p815-p819
crystal
0 0 0
186
3.1900 5.1890
2
231 0.33333333 0.66666667 0.0000
7 0.33333333 0.66666667 0.6230
printout
basisset
end
end
231 9
input
21. 0 2 4 6 2 0
25.880361 370.273040 0
7.901295 9.190615 0
45.149190 99.144001 0
44.979981 198.295512 0
17.224251 28.445653 0
16.747329 56.949705 0
51.968812 -18.168797 0
51.629117 -27.380273 0
15.241738 -1.587022 0
15.320193 -2.516292 0
4.918589 0.083166 0
4.755103 0.202198 0
10.762263 -0.616990 0
19.852939 -3.138584 0
0 0 8 2 1
2848.20 0.000362
420.664 0.002117
29.8118 0.118964
14.2207 -0.461723
2.67643 0.751559
1.13353 0.447202
0.207220 0.012746
0.12 -0.003358
0 0 8 2 1
2848.20 -0.000097
420.664 -0.000614
29.8118 -0.031069
14.2207 0.126784

2.67643 -0.264288
1.13353 -0.275471
0.207220 0.633842
0.12 0.531681
0 0 1 0 1
0.207220 1
0 0 1 0 1
0.12 1
0 2 7 6 1
109.624 0.002101
21.0855 -0.080196
4.92260 0.396415
2.15591 0.519076
0.901913 0.207520
0.202004 0.007825
0.12 -0.001129
0 2 7 1 1
109.624 -0.000288
21.0855 0.013555
4.92260 -0.073629
2.15591 -0.120860
0.901913 -0.001960
0.202004 0.493206
0.12 0.620604
0 2 1 0 1
0.12 1
0 3 7 10 1
85.7978 0.014668
27.6822 0.085621
10.1760 0.248336
3.92208 0.401414
1.45858 0.398604
0.488760 0.186898
0.1772 0.012331
0 3 1 0 1
0.1772 1
7 5
0 0 6 2.0 1.0
6293.4800000 0.00196979
949.0440000 0.0149613
218.7760000 0.0735006
63.6916000 0.2489370
18.8282000 0.6024600
2.7202300 0.2562020
0 1 3 5.0 1.0

30.6331000 0.1119060 0.0383119
7.0261400 0.9216660 0.2374030
2.1120500 -0.00256919 0.8175920
0 1 1 0.0 1.0
0.6840090 1.0000000 1.0000000
0 1 1 0.0 1.0
0.2008780 1.0000000 1.0000000
0 3 1 0.0 1.0
0.9130000 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
end

MnO

MnO – Proceedings of the Japan Academy (1979) 55, p43-p48
CRYSTAL
0 0 0
225
4.4461
2
25 0. 0. 0.
8 0.5 0.5 0.5
PRINTOUT
BASISSET
END
SUPERCEL
0. 1. 1. 1. 0. 1. 1. 1. 0.
END
8 4
0 0 6 2 1
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 6 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8000000 1.0000000
25 8
0 0 6 2 1
56347.1400000 1.771580E-03
8460.9430000 1.357081E-02
1927.3250000 6.690605E-02
543.2343000 2.318541E-01
173.9905000 4.799046E-01
59.3600500 3.495737E-01
0 1 6 8 1
1165.4120000 2.388751E-03 3.977318E-03
277.3276000 3.181708E-02 3.103112E-02
89.4727800 1.254670E-01 1.351894E-01
33.4825600 -2.955431E-02 3.457387E-01

13.5403700 -6.175160E-01 4.629205E-01
5.5579720 -4.544458E-01 2.090592E-01
0 1 6 8 1
45.8353200 -3.665856E-03 -6.887578E-03
15.1877700 7.231971E-02 -2.846816E-02
6.5007100 2.544486E-01 6.031832E-02
2.7515830 -2.910380E-01 3.938961E-01
1.1454040 -7.359860E-01 5.013769E-01
0.4536870 -1.997617E-01 1.792264E-01
0 1 3 2 1
1.7579990 0.05628572 -0.5035024
0.6670220 0.2897491 0.2345011
0.1051290 -1.1406530 0.9141257
0 1 1 0 1
0.1 1.000000E+00 1.00000000
0 3 3 5 1
20.9435500 8.672702E-02
5.5104860 3.841883E-01
1.6650380 7.069071E-01
0 3 1 0 1
0.4617330 1.0000000
0 4 1 0 1
0.8 1.
99 0
END
UHF
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
ATOMSPIN
2
1 1 2 -1
SPINLOCK
0 4
SCFDIR
BIPOSIZE
30000000
EXCHSIZE

30000000
MAXCYCLE
100
FMIXING
60
ANDERSON
PPAN
END

MgTe

MgTe – Journal of Physics: Condensed Matter (2007) 19, p386234-1-p386234-9
crystal
0 0 0
216
6.517
2
12 0. 0. 0.
252 0.25 0.25 0.25
printout
basisset
end
end
12 11
0 0 6 2 1
43866.5000000 0.0009180
6605.3700000 0.0070470
1513.2600000 0.0359410
432.3170000 0.1414610
142.1490000 0.4267640
51.3983000 0.4979750
0 0 3 2 1
51.3983000 0.2513550
19.9196000 0.6186710
8.0247400 0.1884170
0 0 1 2 1
2.5081700 1.0000000
0 0 1 0 1
0.8715310 1.0000000
0 0 1 0 1
0.1081880 1.0000000
0 0 1 0 1
0.08 1.
0 2 4 6 1
193.8540000 0.0101880
45.4420000 0.0753600
14.1864000 0.3074190
5.0575100 0.7175750
0 2 2 0 1
1.8886100 0.6673390
0.7226520 0.3946490
0 2 1 0 1
0.2364170 1.0000000
0 2 1 0 1

0.0933580 1.0000000
0 3 1 0 1
0.1750000 1.0000000
252 6
input
6. 0 2 4 2 2 0
2.656483 50.217674 0
2.281974 1.982941 0
2.946988 39.938015 0
2.790001 79.873384 0
1.750168 -0.651126 0
1.909579 -1.288332 0
1.107233 5.059096 0
1.084059 7.498701 0
1.992613 -7.997183 0
1.968281 -10.464938 0
0 0 3 2 1
4.620870 -0.076259
3.407086 0.222163
1.353795 -0.541514
0 0 1 0 1
0.278218 1.0
0 0 1 0 1
0.128403 1.0
0 2 3 4 1
4.772823 -0.038412
3.508559 0.112992
1.653984 -0.229605
0 2 1 0 1
0.326880 1.0
0 2 1 0 1
0.139746 1.0
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle

100
tolscf
7 7
fmixing
80
broyden
0.0001
end

ZnS

ZnS – Journal of Physics and Chemistry of Solids (1980) 41, p963-p964
crystal
0 0 0
216
5.3829
2
230 0. 0. 0.
16 0.25 0.25 0.25
printout
basisset
end
end
230 10
input
20. 0 2 4 4 2 0
34.174001 399.986399 0
14.456371 85.489750 0
39.888683 92.381077 0
39.655017 184.771176 0
15.290546 23.002541 0
14.903524 46.057427 0
43.708296 -13.690734 0
43.698536 -20.543980 0
15.150718 -1.316154 0
15.282441 -1.838715 0
8.160014 -0.370360 0
12.228422 -1.062943 0
0 0 7 2 1
0.62912600e+03 0.55900000e-03
0.62963500e+02 -0.96800000e-02
0.39579100e+02 0.62354000e-01
0.11917300e+02 -0.41487900e+00
0.25082400e+01 0.75446600e+00
0.10301900e+01 0.45899600e+00
0.15400200e+00 0.11664000e-01
0 0 7 2 1
0.62912600e+03 -0.12100000e-03
0.62963500e+02 0.14890000e-02
0.39579100e+02 -0.12737000e-01
0.11917300e+02 0.97246000e-01
0.25082400e+01 -0.21991700e+00
0.10301900e+01 -0.23647400e+00
0.15400200e+00 0.58129100e+00

0 0 7 0 1
0.62912600e+03 0.42100000e-03
0.62963500e+02 -0.51090000e-02
0.39579100e+02 0.41447000e-01
0.11917300e+02 -0.34164300e+00
0.25082400e+01 0.14386170e+01
0.10301900e+01 -0.98242900e+00
0.15400200e+00 -0.11876310e+01
0 0 1 0 1
0.1 0.10000000e+01
0 2 6 6 1
0.92903400e+02 0.24880000e-02
0.19745200e+02 -0.79136000e-01
0.45507300e+01 0.38805900e+00
0.20019000e+01 0.50935400e+00
0.84387900e+00 0.22457500e+00
0.20338100e+00 0.12680000e-01
0 2 6 0 1
0.92903400e+02 -0.53000000e-03
0.19745200e+02 0.24743000e-01
0.45507300e+01 -0.14247800e+00
0.20019000e+01 -0.23403200e+00
0.84387900e+00 0.92187000e-01
0.20338100e+00 0.83777000e+00
0 2 1 0 1
0.59572000e-01 0.10000000e+01
0 3 6 10 1
0.71276600e+02 0.15895000e-01
0.22760400e+02 0.92454000e-01
0.83236900e+01 0.25947200e+00
0.31687500e+01 0.40331400e+00
0.11470300e+01 0.38783400e+00
0.36664300e+00 0.20225800e+00
0 3 6 0 1
0.71276600e+02 -0.22516000e-01
0.22760400e+02 -0.13330300e+00
0.83236900e+01 -0.39325300e+00
0.31687500e+01 -0.35121400e+00
0.11470300e+01 0.40617100e+00
0.36664300e+00 0.57920500e+00
0 3 1 0 1
0.36664300e+00 0.10000000e+01
16 12
0 0 6 2 1
93413.4000000 0.0007430

13961.7000000 0.0057930
3169.9100000 0.0299540
902.4560000 0.1190280
297.1580000 0.3684320
108.7020000 0.5772990
0 0 3 2 1
108.7020000 0.1431860
43.1553000 0.6244650
18.1079000 0.2833660
0 0 1 2 1
5.5600900 1.0000000
0 0 1 0 1
2.1318300 1.0000000
0 0 1 0 1
0.4204030 1.0000000
0 0 1 0 1
0.1360450 1.0000000
0 2 4 6 1
495.0400000 0.0083090
117.2210000 0.0640240
37.7749000 0.2776140
14.0584000 0.7450760
0 2 2 4 1
5.5657400 0.6137120
2.2629700 0.4438180
0 2 1 0 1
0.8079940 1.0000000
0 2 1 0 1
0.2774600 1.0000000
0 2 1 0 1
0.1 1.
0 3 1 0 1
0.6500000 1.0000000
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24

```
maxcycle
100
fmixing
80
tolscf
7 7
broyden
0.0001
end
```

CuSCN

beta-cuscn – acta crystallographica b (24,1968-38,1982) (1981) 37, p1807-p1812
crystal
0 0 0
160
3.856 32.905
8
229 0.0000 0.0000 0.0000
229 0.0000 0.0000 0.5000
7 0.0000 0.0000 0.0585
7 0.0000 0.0000 0.5585
6 0.0000 0.0000 0.0934
6 0.0000 0.0000 0.5934
16 0.0000 0.0000 0.1445
16 0.0000 0.0000 0.6445
printout
basisset
end
end
229 10
input
19. 0 2 4 4 2 0
30.110543 355.750512 0
13.076310 70.930906 0
32.692614 77.969931 0
32.770339 155.927448 0
13.751067 18.021132 0
13.322166 36.094372 0
38.996511 -12.343410 0
39.539788 -18.273362 0
12.287511 -0.984705 0
11.459300 -1.318747 0
6.190102 -0.227264 0
8.118780 -0.468773 0
0 0 7 2 1
0.56008800e+03 0.63700000e-03
0.56648600e+02 -0.97350000e-02
0.35425800e+02 0.65793000e-01
0.11054600e+02 -0.41503500e+00
0.23068200e+01 0.74661100e+00
0.95142900e+00 0.46217300e+00
0.14518400e+00 0.15983000e-01
0 0 7 1 1
0.56008800e+03 -0.13600000e-03

0.56648600e+02 0.14010000e-02
0.35425800e+02 -0.13174000e-01
0.11054600e+02 0.95695000e-01
0.23068200e+01 -0.21187400e+00
0.95142900e+00 -0.23594400e+00
0.14518400e+00 0.50811500e+00
0 0 7 0 1
0.56008800e+03 -0.33300000e-03
0.56648600e+02 0.59300000e-02
0.35425800e+02 -0.32549000e-01
0.11054600e+02 0.21107100e+00
0.23068200e+01 -0.73055600e+00
0.95142900e+00 0.17724200e+00
0.14518400e+00 0.17148730e+01
0 0 1 0 1
0.12 0.10000000e+01
0 2 6 6 1
0.70973900e+02 0.36820000e-02
0.17851000e+02 -0.82128000e-01
0.42467900e+01 0.37537900e+00
0.18776000e+01 0.50840900e+00
0.79333500e+00 0.23909500e+00
0.19347600e+00 0.15850000e-01
0 2 6 0 1
0.70973900e+02 -0.62800000e-03
0.17851000e+02 0.16563000e-01
0.42467900e+01 -0.84572000e-01
0.18776000e+01 -0.14128300e+00
0.79333500e+00 -0.35710000e-02
0.19347600e+00 0.51900500e+00
0 2 1 0 1
0.12 0.10000000e+01
0 3 6 10 1
0.60380400e+02 0.17564000e-01
0.19112100e+02 0.99134000e-01
0.69528800e+01 0.27117100e+00
0.26099400e+01 0.40618000e+00
0.92256700e+00 0.38142700e+00
0.28364200e+00 0.20062600e+00
0 3 6 0 1
0.60380400e+02 -0.22286000e-01
0.19112100e+02 -0.12827400e+00
0.69528800e+01 -0.36279700e+00
0.26099400e+01 -0.32572200e+00
0.92256700e+00 0.32708700e+00

0.28364200e+00 0.65680900e+00
0 3 1 0 1
0.28364200e+00 0.10000000e+01
16 11
0 0 6 2 1
93413.4000000 0.0007430
13961.7000000 0.0057930
3169.9100000 0.0299540
902.4560000 0.1190280
297.1580000 0.3684320
108.7020000 0.5772990
0 0 3 2 1
108.7020000 0.1431860
43.1553000 0.6244650
18.1079000 0.2833660
0 0 1 2 1
5.5600900 1.0000000
0 0 1 0 1
2.1318300 1.0000000
0 0 1 0 1
0.4204030 1.0000000
0 0 1 0 1
0.1360450 1.0000000
0 2 4 6 1
495.0400000 0.0083090
117.2210000 0.0640240
37.7749000 0.2776140
14.0584000 0.7450760
0 2 2 4 1
5.5657400 0.6137120
2.2629700 0.4438180
0 2 1 0 1
0.8079940 1.0000000
0 2 1 0 1
0.2774600 1.0000000
0 3 1 0 1
0.6500000 1.0000000
6 5
0 0 6 2.0 1.0
4563.2400000 0.00196665
682.0240000 0.0152306
154.9730000 0.0761269
44.4553000 0.2608010
13.0290000 0.6164620
1.8277300 0.2210060

0 1 3 4.0 1.0
20.9642000 0.1146600 0.0402487
4.8033100 0.9199990 0.2375940
1.4593300 -0.00303068 0.8158540
0 1 1 0.0 1.0
0.4834560 1.0000000 1.0000000
0 1 1 0.0 1.0
0.1455850 1.0000000 1.0000000
0 3 1 0.0 1.0
0.6260000 1.0000000
7 5
0 0 6 2.0 1.0
6293.4800000 0.00196979
949.0440000 0.0149613
218.7760000 0.0735006
63.6916000 0.2489370
18.8282000 0.6024600
2.7202300 0.2562020
0 1 3 5.0 1.0
30.6331000 0.1119060 0.0383119
7.0261400 0.9216660 0.2374030
2.1120500 -0.00256919 0.8175920
0 1 1 0.0 1.0
0.6840090 1.0000000 1.0000000
0 1 1 0.0 1.0
0.2008780 1.0000000 1.0000000
0 3 1 0.0 1.0
0.9130000 1.0000000
99 0
end
uhf
dft
b3pw
end
tolinteg
7 7 7 7 14
end
6 0 12
maxcycle
60
tolscf
7 7
fmixing
80
broyden

0.01
end

NiO

NiO – Proceedings of the Japan Academy (1979) 55, p43-p48
CRYSTAL
0 0 0
225
4.178
2
28 0. 0. 0.
8 0.5 0.5 0.5
PRINTOUT
BASISSET
END
SUPERCEL
0. 1. 1. 1. 0. 1. 1. 1. 0.
END
8 4
0 0 6 2 1
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 6 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
28 8
0 0 6 2 1
71396.3500000 1.753003E-03
10720.8400000 1.343122E-02
2442.1290000 6.627041E-02
688.4265000 2.302508E-01
220.6153000 4.790186E-01
75.3937300 3.523444E-01
0 1 6 8 1
1492.5320000 2.370714E-03 3.967554E-03
355.4013000 3.160566E-02 3.109479E-02
114.9534000 1.266335E-01 1.359517E-01
43.2204300 -2.417037E-02 3.485136E-01

17.5971000 -6.187775E-01 4.625498E-01
7.2577650 -4.576770E-01 2.035186E-01
0 1 6 8 1
59.3526100 -4.162002E-03 -7.421452E-03
20.0218100 7.425111E-02 -2.953410E-02
8.6145610 2.541360E-01 6.731852E-02
3.6605310 -2.903477E-01 4.016660E-01
1.5281110 -7.302121E-01 4.926623E-01
0.6040570 -2.076057E-01 1.756893E-01
0 1 3 2 1
2.3792760 0.05157888 -0.1887663
0.8858390 0.2707611 0.1015199
0.1285290 -1.1247700 0.9790906
0 1 1 0 1
0.1 1.000000E+00 1.00000000
0 3 3 8 1
28.1914700 9.098881E-02
7.5235840 3.958208E-01
2.2712280 6.947154E-01
0 3 1 0 1
0.611603 1.0000000
0 4 1 0 1
0.8 1.
99 0
END
UHF
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
ATOMSPIN
2
1 1 2 -1
SPINLOCK
0 8
SCFDIR
BIPOSIZE
30000000
EXCHSIZE

30000000
MAXCYCLE
100
FMIXING
60
ANDERSON
PPAN
END

AlN (zincblende)

AlN (zincblende) – Physical Review, Serie 3. B - Condensed Matter (18,1978-) (1995) 51, p7866-p7869
CRYSTAL
0 0 0
216
4.3420
2
13 0.00 0.00 0.0000
7 0.25 0.25 0.25
PRINTOUT
BASISSET
END
END
13 5
0 0 6 2 1
13983.1000000 0.00194267
2098.7500000 0.0148599
477.7050000 0.0728494
134.3600000 0.2468300
42.8709000 0.4872580
14.5189000 0.3234960
0 1 6 8 1
239.6680000 -0.00292619 0.00460285
57.4419000 -0.0374080 0.0331990
18.2859000 -0.1144870 0.1362820
6.5991400 0.1156350 0.3304760
2.4904900 0.6125950 0.4491460
0.9445400 0.3937990 0.2657040
0 1 3 3 1
1.2779000 -0.2276060 -0.0175130
0.3975900 0.00144583 0.2445330
0.1600950 1.0927900 0.8049340
0 1 1 0 1
0.1 1. 1.
0 3 1 0 1
0.325 1.0
7 5
0 0 6 2 1
6293.4800000 0.00196979
949.0440000 0.0149613
218.7760000 0.0735006
63.6916000 0.2489370
18.8282000 0.6024600

2.7202300 0.2562020
0 1 3 5 1
30.6331000 0.1119060 0.0383119
7.0261400 0.9216660 0.2374030
2.1120500 -0.00256919 0.8175920
0 1 1 0 1
0.6840090 1.0000000 1.0000000
0 1 1 0 1
0.2008780 1.0000000 1.0000000
0 3 1 0 1
0.9130000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

C (Diamond)

C diamond– Acta Crystallographica. Section A: Foundations of Crystallography (2014) 70, (1) p39-p48
CRYSTAL
0 0 0
227
3.5666
1
6 0.1250 0.1250 0.1250
PRINTOUT
BASISSET
END
END
6 5
0 0 6 2.0 1.0
4563.2400000 0.00196665
682.0240000 0.0152306
154.9730000 0.0761269
44.4553000 0.2608010
13.0290000 0.6164620
1.8277300 0.2210060
0 1 3 4.0 1.0
20.9642000 0.1146600 0.0402487
4.8033100 0.9199990 0.2375940
1.4593300 -0.00303068 0.8158540
0 1 1 0.0 1.0
0.4834560 1.0000000 1.0000000
0 1 1 0.0 1.0
0.1655850 1.0000000 1.0000000
0 3 1 0.0 1.0
0.6260000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 9 30
TOLDEE
7
SHRINK
12 0 24
SCFDIR

BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
END

AlN (Wurtzite)

AlN– Solid State Communications (1977) 23, p815-p819
CRYSTAL
0 0 0
186
3.1100 4.9800
2
13 0.33333333 0.66666667 0.0000
7 0.33333333 0.66666667 0.6179
PRINTOUT
BASISSET
END
END
13 5
0 0 6 2 1
13983.1000000 0.00194267
2098.7500000 0.0148599
477.7050000 0.0728494
134.3600000 0.2468300
42.8709000 0.4872580
14.5189000 0.3234960
0 1 6 8 1
239.6680000 -0.00292619 0.00460285
57.4419000 -0.0374080 0.0331990
18.2859000 -0.1144870 0.1362820
6.5991400 0.1156350 0.3304760
2.4904900 0.6125950 0.4491460
0.9445400 0.3937990 0.2657040
0 1 3 3 1
1.2779000 -0.2276060 -0.0175130
0.3975900 0.00144583 0.2445330
0.1600950 1.0927900 0.8049340
0 1 1 0 1
0.1 1. 1.
0 3 1 0 1
0.325 1.0
7 5
0 0 6 2 1
6293.4800000 0.00196979
949.0440000 0.0149613
218.7760000 0.0735006
63.6916000 0.2489370
18.8282000 0.6024600
2.7202300 0.2562020

0 1 3 5 1
30.6331000 0.1119060 0.0383119
7.0261400 0.9216660 0.2374030
2.1120500 -0.00256919 0.8175920
0 1 1 0 1
0.6840090 1.0000000 1.0000000
0 1 1 0 1
0.2008780 1.0000000 1.0000000
0 3 1 0 1
0.9130000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

BN

BN – Journal of Physics and Chemistry of Solids (1990) 51, (8) p1011-p1012
CRYSTAL
0 0 0
216
3.616
2
5 0.0000 0.0000 0.0000
7 0.25 0.25 0.25
PRINTOUT
BASISSET
END
END
5 5
0 0 6 2 1
2858.8900000 0.00215375
428.1400000 0.0165823
97.5282000 0.0821870
27.9693000 0.2766180
8.2157700 0.6293160
1.1127800 0.1737700
0 1 3 3 1
13.2415000 0.1174430 0.0418100
3.0016600 0.9180020 0.2365750
0.9128560 -0.00265105 0.8162140
0 1 1 0 1
0.3154540 1.0000000 1.0000000
0 1 1 0 1
0.12 1.0000000 1.0000000
0 3 1 0 1
0.4010000 1.0000000
7 5
0 0 6 2.0 1.0
6293.4800000 0.00196979
949.0440000 0.0149613
218.7760000 0.0735006
63.6916000 0.2489370
18.8282000 0.6024600
2.7202300 0.2562020
0 1 3 5.0 1.0
30.6331000 0.1119060 0.0383119
7.0261400 0.9216660 0.2374030
2.1120500 -0.00256919 0.8175920
0 1 1 0.0 1.0

0.6840090 1.0000000 1.0000000
0 1 1 0.0 1.0
0.2008780 1.0000000 1.0000000
0 3 1 0.0 1.0
0.9130000 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 9 30
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

MgO

MGO – ACTA CRYSTALLOGRAPHICA, SECTION B: STRUCTURAL SCIENCE (1998) 54, P8-P17
CRYSTAL
0 0 0
225
4.214
2
12 0. 0. 0.
8 0.5 0.5 0.5
PRINTOUT
BASISSET
END
END
12 10
0 0 6 2 1
43866.5000000 0.0009180
6605.3700000 0.0070470
1513.2600000 0.0359410
432.3170000 0.1414610
142.1490000 0.4267640
51.3983000 0.4979750
0 0 3 2 1
51.3983000 0.2513550
19.9196000 0.6186710
8.0247400 0.1884170
0 0 1 2 1
2.5081700 1.0000000
0 0 1 0 1
0.8715310 1.0000000
0 0 1 0 1
0.1081880 1.
0 2 4 6 1
193.8540000 0.0101880
45.4420000 0.0753600
14.1864000 0.3074190
5.0575100 0.7175750
0 2 2 0 1
1.8886100 0.6673390
0.7226520 0.3946490
0 2 1 0 1
0.2364170 1.0000000
0 2 1 0 1
0.1 1.

0 3 1 0 1
0.1750000 1.0000000
8 4
0 0 6 2 1
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 6 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
99 0
END
UHF
DFT
B3PW
END
TOLINTEG
7 7 7 9 30
TOLDEE
7
SHRINK
12 0 24
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

NaCl

NaCl – Inorganic Chemistry (2006) 45, P7367-P7371
CRYSTAL
0 0 0
225
5.6573
2
11 0.00 0.00 0.00
17 0.5 0.5 0.5
PRINTOUT
BASISSET
END
END
11 10
0 0 6 2 1
36166.4000000 0.0010320
5372.5800000 0.0080710
1213.2100000 0.0421290
339.6230000 0.1697890
109.5530000 0.5146210
38.7773000 0.3798170
0 0 3 2 1
38.7773000 0.3747620
14.5759000 0.5757690
5.2699300 0.1129330
0 0 1 1 1
1.8277700 1.0000000
0 0 1 0 1
0.6199480 1.0000000
0 0 1 0 1
0.10 1.0000000
0 2 4 6 1
144.6450000 0.0114850
33.9074000 0.0823830
10.6285000 0.3196580
3.8238900 0.7012950
0 2 2 0 1
1.4442900 0.6385060
0.5526210 0.4253650
0 2 1 0 1
0.1887200 1.0000000
0 2 1 0 1
0.10 1.0000000
0 3 1 0 1

0.1750000 1.0000000
17 12
0 0 6 2 1
105819.0000000 0.0007380
15872.0000000 0.0057180
3619.6500000 0.0294950
1030.8000000 0.1172860
339.9080000 0.3629490
124.5380000 0.5841490
0 0 3 2 1
124.5380000 0.1341770
49.5135000 0.6242500
20.8056000 0.2917560
0 0 1 2 1
6.5834600 1.0000000
0 0 1 0 1
2.5646800 1.0000000
0 0 1 0 1
0.5597630 1.0000000
0 0 1 0 1
0.1832730 1.0000000
0 2 5 6 1
589.7760000 0.0023910
139.8490000 0.0185040
45.1413000 0.0813770
16.8733000 0.2215520
6.7411000 0.7725690
0 2 2 5 1
6.7411000 -1.5722440
2.7715200 0.9923890
0 2 1 0 1
1.0238700 1.0000000
0 2 1 0 1
0.3813680 1.0000000
0 2 1 0 1
0.1094370 1.0000000
0 3 1 0 1
0.7500000 1.0000000
99 0
END
DFT
B3PW
END
TOLINTEG
7 7 7 7 14

EXCHSIZE
8000000
BIPOSIZE
8000000
SHRINK
24 48
MAXCYCLE
200
FMIXING
60
ANDERSON
NODIRECT
END

SiO_2 (β-cristobalite)

SiO2: beta-cristobalite– Zeitschrift fuer Kristallographie (1979-2010) (1992) 201, p125-p145
CRYSTAL
0 0 0
227
7.12637
2
14 0.1250 0.1250 0.1250
8 0.0000 0.0000 0.0000
PRINTOUT
BASISSET
END
END
14 12
0 0 6 2 1
69379.2300000 0.0007570
10354.9400000 0.0059320
2333.8796000 0.0310880
657.1429500 0.1249670
214.3011300 0.3868970
77.6291680 0.5548880
0 0 3 2 1
77.6291680 0.1778810
30.6308070 0.6277650
12.8012950 0.2476230
0 0 1 2 1
3.9268660 1.0000000
0 0 1 0 1
1.4523430 1.0000000
0 0 1 0 1
0.2562340 1.0000000
0 0 1 0 1
0.12 1.0000000
0 2 4 6 1
335.4831900 0.0088660
78.9003660 0.0682990
24.9881500 0.2909580
9.2197110 0.7321170
0 2 2 2 1
3.6211400 0.6198790
1.4513100 0.4391480
0 2 1 0 1
0.5049770 1.0000000
0 2 1 0 1

0.1863170 1.0000000
0 2 1 0 1
0.12 1.0000000
0 3 1 0 1
0.4500000 1.0000000
8 4
0 0 6 2 1
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 6 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
NODIRECT

END

LiCl

LiCl – Proceedings of the Physical Society, London (1936) 48, p85-p94
CRYSTAL
0 0 0
225
5.146
2
3 0.00 0.00 0.00
17 0.5 0.5 0.5
PRINTOUT
BASISSET
END
END
3 4
0 0 6 2 1
900.4600000 0.00228704
134.4330000 0.0176350
30.4365000 0.0873434
8.6263900 0.2809770
2.4833200 0.6587410
0.3031790 0.1187120
0 1 3 1 1
4.8689000 0.0933293 0.0327661
0.8569240 0.9430450 0.1597920
0.2432270 -0.00279827 0.8856670
0 1 1 0 1
0.12 1. 1.
0 3 1 0 1
0.2 1. 1.
17 12
0 0 6 2 1
105819.0000000 0.0007380
15872.0000000 0.0057180
3619.6500000 0.0294950
1030.8000000 0.1172860
339.9080000 0.3629490
124.5380000 0.5841490
0 0 3 2 1
124.5380000 0.1341770
49.5135000 0.6242500
20.8056000 0.2917560
0 0 1 2 1
6.5834600 1.0000000
0 0 1 0 1

2.5646800 1.0000000
0 0 1 0 1
0.5597630 1.0000000
0 0 1 0 1
0.1832730 1.0000000
0 2 5 6 1
589.7760000 0.0023910
139.8490000 0.0185040
45.1413000 0.0813770
16.8733000 0.2215520
6.7411000 0.7725690
0 2 2 5 1
6.7411000 -1.5722440
2.7715200 0.9923890
0 2 1 0 1
1.0238700 1.0000000
0 2 1 0 1
0.3813680 1.0000000
0 2 1 0 1
0.1094370 1.0000000
0 3 1 0 1
0.7500000 1.0000000
99 0
END
DFT
B3PW
END
TOLINTEG
7 7 7 7 14
EXCHSIZE
8000000
BIPOSIZE
8000000
SHRINK
12 24
MAXCYCLE
200
FMIXING
60
ANDERSON
NODIRECT
END

SiO2 (α-quartz)

SiO2– Materials Letters (2006) 60, p3526-p3529
CRYSTAL
0 0 0
152
4.9210 5.400
2
14 0.5280 0.0000 0.3333
8 0.4080 0.1430 0.1193
PRINTOUT
BASISSET
END
END
14 12
0 0 6 2 1
69379.2300000 0.0007570
10354.9400000 0.0059320
2333.8796000 0.0310880
657.1429500 0.1249670
214.3011300 0.3868970
77.6291680 0.5548880
0 0 3 2 1
77.6291680 0.1778810
30.6308070 0.6277650
12.8012950 0.2476230
0 0 1 2 1
3.9268660 1.0000000
0 0 1 0 1
1.4523430 1.0000000
0 0 1 0 1
0.2562340 1.0000000
0 0 1 0 1
0.12 1.0000000
0 2 4 6 1
335.4831900 0.0088660
78.9003660 0.0682990
24.9881500 0.2909580
9.2197110 0.7321170
0 2 2 2 1
3.6211400 0.6198790
1.4513100 0.4391480
0 2 1 0 1
0.5049770 1.0000000
0 2 1 0 1

0.1863170 1.0000000
0 2 1 0 1
0.12 1.0000000
0 3 1 0 1
0.4500000 1.0000000
8 4
0 0 6 2 1
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
0 1 3 6 1
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0 1 1 0 1
0.2700058 1.0000000 1.0000000
0 3 1 0 1
0.8 1.0000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEG
7 7 7 7 14
TOLDEE
7
SHRINK
12 0 24
SCFDIR
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
15
FMIXING
60
ANDERSON
PPAN
NODIRECT

END

LiF

LiF – Kristallografiya (1988) 33, p90-p97
CRYSTAL
0 0 0
225
4.027
2
9 0.00 0.00 0.00
3 0.5 0.5 0.5
PRINTOUT
BASISSET
END
END
3 10
0 0 9 2 1
5988.0000000 0.0001330
898.9000000 0.0010250
205.9000000 0.0052720
59.2400000 0.0209290
19.8700000 0.0663400
7.4060000 0.1657750
2.9300000 0.3150380
1.1890000 0.3935230
0.4798000 0.1908700
0 0 9 1 1
5988.0000000 -0.0000210
898.9000000 -0.0001610
205.9000000 -0.0008200
59.2400000 -0.0033260
19.8700000 -0.0105190
7.4060000 -0.0280970
2.9300000 -0.0559360
1.1890000 -0.0992370
0.4798000 -0.1121890
0 0 1 0 1
1.9740000 1.0000000
0 0 1 0 1
0.6830000 1.0000000
0 2 3 0 1
3.2660000 0.0086300
0.6511000 0.0475380
0.1696000 0.2097720
0 2 1 0 1
7.3200000 1.0000000

0 2 1 0 1
1.8750000 1.0000000
0 3 1 0 1
0.1874000 1.0000000
0 3 1 0 1
4.9120000 1.0000000
0 4 1 0 1
0.1829000 1.0000000
9 4
0 0 6 2 1
7001.7130900 0.0018196169
1051.3660900 0.0139160796
239.2856900 0.0684053245
67.3974453 0.233185760
21.5199573 0.471267439
7.40310130 0.356618546
0 1 3 7 1
20.8479528 -0.108506975 0.0716287243
4.80830834 -0.146451658 0.3459121030
1.34406986 1.128688580 0.7224699570
0 1 1 0 1
0.358151393 1.0000000 1.0000000
0 3 1 0 1
0.8000000 1.0000000
99 0
END
DFT
B3PW
END
TOLINTEG
7 7 7 7 14
TOLDEE
7 7
EXCHSIZE
8000000
BIPOSIZE
8000000
SHRINK
12 24
MAXCYCLE
30
FMIXING
60
ANDERSON
END