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.\textsuperscript{[1]}

- 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$_2$Se$_3$ 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)
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.

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<th>PBE</th>
<th>GW</th>
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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.

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S19
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.

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<th>PBE</th>
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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.

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S22
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<td>BN</td>
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<td>?</td>
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</tr>
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<td>S97</td>
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<td>0 (extrapolated)</td>
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<td>?</td>
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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$_2$Te$_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 $\sim 0.01$ eV and the MADs for B3PW increased by $\sim 0.01$ 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.
References


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$_2$Se$_3$ (6q)**

bi2se3 – Inorg Chem (1999) 38 (9) 2131

crystal
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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
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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
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1.248042 -0.912045
0.365482 -0.259603
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0.270727 1.0
0 0 1 0 1

S32
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0.555533 -0.317612
0.411224 0.38604
0.2101
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
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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
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 0.001829
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
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1.5894 -0.364598
0.3830 0.698440
0.1399 0.532390
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0.3830 1
0 0 1 0. 1
0.1399 1
0 2 7 6.0 1
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25.8909 -0.084899
6.2093 0.428655
2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
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2.6613 -0.193545
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0.3597 0.591806
0.1137 0.499759
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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
fmethod
80
broyden
0.01
ppan
end
\textbf{Bi}_2\textbf{Se}_3 (7QL)

\textit{Bi}_2\textit{Se}_3 – 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

S36
0.165982 1.0
0.2101
0.077856 1.0
0.3101
0.256 1.0
0.3101
0.134 1.0
234 9
input
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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 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 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 8 2.0 1
0 8 2.0 1
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0.3830 1
0 0 1 0. 1
0.1399 1
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2.6613 0.543060
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0.1137 0.001019
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
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128.508 0.011011
41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
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0.3656 1
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end
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dft
b3pw
end
biesplit
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tolinteg
977714
end
10 0 20
maxcycle
20
fmixing
80
broyden
0.01
ppan
end
Bi

bi – Acta Crystallographica 1962 15 865

crystal

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166

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1

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end

283 9

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6.252592 9.991550 0

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tolpseud
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end
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maxcycle
100
fmixing
80
broyden
0.0001
tolscf
8 8
ppan
end
Bi$_2$Se$_3$ (5QL)

bi2se3 – Inorg Chem (1999) 38 (9) 2131

crystal
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166
4.1355 28.615
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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
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0.875463 5.715603 0
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0.232846 -0.150845 0
0.797775 4.060445 0
0.739216 5.980282 0
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0.959907 -3.373825 0
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1.696224 0.519113
1.248042 -0.912045
0.365482 -0.259603
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0.120284 1.0
0 2 3 3 1
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0.555533 -0.317612
0.411224 0.38604
0 2 1 0 1
| 0.165982 | 1.0 |
| 0.2101 | 1.0 |
| 0.077856 | 1.0 |
| 0.3101 | 1.0 |
| 0.256 | 1.0 |
| 0.3101 | 1.0 |
| 0.134 | 1.0 |
| 234 | 9 |

input

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| 45.294642 | 198.292483 | 0 |
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| 20.028601 | 56.749747 | 0 |
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| 17.810780 | -2.102742 | 0 |
| 008201 |
| 2609.7204 | 0.001829 |
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| 48.2893 | 0.071606 |
| 16.8019 | -0.383980 |
| 3.5149 | 0.691926 |
| 1.5894 | 0.491893 |
| 0.3830 | 0.021091 |
| 0.1399 | -0.003916 |
| 008201 |
| 2609.7204 | -0.000694 |
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| 0.3830 | 0.698440 |
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| 00101 |
| 0.3830 | 1 |
| 00101 |

S44
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0.1137 0.001019
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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
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uhf
dft
b3pw
end
biesplit
10
tolinteg
9 7 7 7 14
end
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maxcycle
20
fmixing
80
broyden

S45
0.01
ppan
end
\textbf{Bi}_2\textbf{Se}_3 \ (4QL)

\textit{bi2se3} \ – Inorg Chem (1999) 38 (9) 2131

crystal
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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
0.797775 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
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0.555533 -0.317612
0.411224 0.38604
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2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
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
0.210. 1
0.1137 1
0.3656 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
0.310. 1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
977714
end
10 020
maxcycle
20
fmixing
80
broyden
0.01
ppan
end
**Bi$_2$Se$_3$ (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
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0.365482 -0.259603
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0.411224 0.38604
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0.077856 1.0
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0.256 1.0
0 3 1 0 1
0.134 1.0
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45.294642 198.292483 0
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20.028601 56.749747 0
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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
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391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
3.5149 0.691926
1.5894 0.491893
0.3830 0.698440
0.1399 0.532390
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S52
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0.1137 0.001019
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0.3610.1
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41.5212 0.077856
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6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
0.310.1
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end
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dft
b3pw
end
biesplit
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tolinteg
977714
end
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maxcycle
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fmixing
80
broyden
Bi$_2$Se$_3$

bi2se3 – Inorg Chem (1999) 38 (9) 2131

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234 0.000 0.000 0.2109  

end  
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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  
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0.365482 -0.259603  
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0 0 1 0 1  
0.120284 1.0  
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0.165982 1.0  
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0 3 1 0 1  
0.134 1.0  

S55
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45.294642 198.292483 0
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20.028601 56.749747 0
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3.501953 0.235583 0
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17.810780 -2.102742 0
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2609.7204 0.001829
391.5228 0.009706
48.2893 0.071606
16.8019 -0.383980
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1.5894 0.491893
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48.2893 -0.024839
16.8019 0.140207
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0.3597 0.591806
0.1137 0.499759
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0 3 6 10. 1
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41.5212 0.077856
15.5182 0.232819
6.16082 0.401788
2.41134 0.408946
0.871936 0.168093
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end
uhf
dft
b3pw
end
biesplit
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tolinteg
9 7 7 7 14
df
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maxcycle
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fmixing
80
broyden
0.01
end
PbSe


crystal

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printout

basisset
end
end
282 8

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0.256555 -0.151563 0
0.189112 -0.090292 0
0.664793 2.956364 0
0.621886 4.242489 0
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0.779307 -2.666379 0
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0.340937 -0.298476
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0 0 1 0 1
0.109434 1.0
0 2 3 2 0 1
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0.604749 -0.206213
0.442006 0.173019
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0.180638 1.0
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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
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20.028601 56.749747 0
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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
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0.3830 1
0 0 1 0. 1
0.1399 1
0 2 7 6.0 1
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6.2093 0.428655
Bi₂Te₃

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252 0.000 0.000 0.2097
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basisset
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end
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0.232846 -0.150845 0
0.779775 4.060445 0
0.739216 5.98028 0
0.987519 -2.646547 0
0.959907 -3.373825 0
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1.248042 -0.912045
0.365482 -0.259603
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0.120284 1.0
0 2 3 3 1
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dft
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end
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maxcycle
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S62
fmixing
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ppan
end
PbTe

PbTe – Acta Crystallographica, Section B: Structural Science (1983) 39, p312-p317

crystal

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S64
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1.107233 5.059096 0
1.084059 7.498701 0
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1.968281 -10.464938 0
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0.278218 1.0
0 0 1 0 1
0.128403 1.0
0 2 3 4 1
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0.326880 1.0
0 2 1 0 1
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dft
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end
biesplit
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broyden
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tolscf
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InSb

InSb – Materials Chemistry and Physics (2008) 112, p745-p748

Crystal
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12.552561 -18.206866 0
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2.08201 -0.180749
0.844314 -0.114582
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0.1 0.687789
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0.1 1
0 3 6 10 1
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8.092728 29.518512 0
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end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.001
end
end
**Bi$_2$Se$_3$ (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
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Crystal

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InN (wurtzite) – Powder Diffraction (2003) 18, p114-p121

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Si– Materials Science Forum (2001) 378, p288-p293

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B3PW
XLGRID
END
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TOLDEE 7
SHRINK 12 0 24
SCFDIR
BIPOSEIZE 30000000
EXCHSIZE 30000000
MAXCYCLE 50
FMIXING 60
ANDERSON PPAN
NODIRECT
END
MoS2


crystal
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194
3.1602 12.2940
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16 0.33333333 0.66666667 0.6210

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end
end
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4.375670 24.715920 0
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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
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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
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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
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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 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
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0.12 0.10000000E+01
0 3 5 4 1
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0.21046200E+01 0.13198200E+00
0.95820100E+00 0.34708600E+00
0.41404700E+00 0.40547100E+00
0.16845000E+00 0.28805800E+00
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0.21046200E+01 -0.16062100E+00
0.95820100E+00 -0.42322900E+00
0.41404700E+00 -0.19233900E+00
0.16845000E+00 0.53145900E+00
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0.12 0.10000000E+01
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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
S107
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43.1553000 0.6244650
18.1079000 0.2833660
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2.1318300 1.0000000
0 0 1 0 1
0.4204030 1.0000000
0 0 1 0 1
0.1360450 1.0000000
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117.2210000 0.0640240
37.7749000 0.2776140
14.0584000 0.7450760
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5.5657400 0.6137120
2.2629700 0.4438180
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0.8079940 1.0000000
0 2 1 0 1
0.2774600 1.0000000
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0.12 1.
0 3 1 0 1
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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


crystal

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216
5.869
2
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15 0.25 0.25 0.25

printout
basisset
end
end
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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 -0.296647
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

S111
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
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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
dend
uhf
dft
b3pw
dend
biesplit
10
tolinteg
7 7 7 7 14
dend
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.01
dend

S112
GaAs


crystal

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216
5.6521
2
231 0 0 0
233 0.25 0.25 0.25

printout

basisset

end

end

231 9

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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
1.13353 0.447202
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

S113
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0.1 0.531681
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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
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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
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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
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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
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381.169 -0.002190
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0.318424 0.005764
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0 2 7 3 1
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0.100972 0.535653
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0.100972 1
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13.6893 0.236755
5.38964 0.401534
2.08046 0.406686
0.737568 0.173162
0.3078 0.008730
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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
fmxing
80
broyden
0.01
end
CdTe

CdTe – Kristallografiya (2001) 46, (4) p703-p709

Crystal

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216
6.4827
2
248 0.000 0.000 0.000
252 0.25 0.25 0.25

printout

basisset
end

end
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6.400743 21.265046 0
11.161722 31.663965 0
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4.537733 5.186200 0
4.335727 7.566063 0
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11.487027 -16.760171 0
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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
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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

S117
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0.14652200e+02 0.28897500e+00
0.65704440e+01 -0.73154600e+00
0.15378300e+01 0.19768990e+01
0.69098400e+00 -0.73154600e+00
0.13491300e+00 -0.11186740e+01
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0.07 0.10000000e+01
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0.21182000e+01 0.53527400e+00
0.98926200e+00 0.49636200e+00
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0.13916000e+00 0.32100000e-02
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0.84632200e+01 0.10874400e+00
0.21182000e+01 -0.27823100e+00
0.98926200e+00 -0.32939000e+00
0.43178100e+00 0.35463000e+00
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0.09 0.10000000e+01
0 3 6 1 0
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0.12221400e+02 -0.11791000e-01
0.31219900e+01 0.24119400e+00
0.13894100e+01 0.44898000e+00
0.57320300e+00 0.38021100e+00
0.21170800e+00 0.14453000e+00
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0.57320300e+00 0.57146200e+00
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<td>1</td>
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<td>6</td>
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0 3 6 10. 1
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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


crystal
0 0 0
216
6.0959
2
13 0. 0. 0.
251 0.25 0.25 0.25
printout
basisset
end
end
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0 0 6 2 1
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2098.750000 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
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0 1 3 3 1
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0.1600950 1.0927900 0.8049340
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14.470337 67.457380 0
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99
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
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end
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end
end
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0.13491300e+00 0.61353300e+00

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16.323522 -0.696089 0
14.465196 -1.167891 0
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17.810780 -2.102742 0
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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
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391.5228 -0.003866
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2.6613 0.543060
1.0929 0.149283
0.3597 0.001071
0.1137 0.001019
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1.0929 0.047373
0.1137 0.499759
0.210.1
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
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uhf
dft
b3pw
end
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
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broyden
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BP


CRYSTAL
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END
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11605.8000000 0.0060680
2645.9600000 0.0311600
754.9760000 0.1234310
248.7550000 0.3782090
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S128


Cu$_2$O


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end
end
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32.770339 155.927448 0
13.751067 18.021132 0
13.322166 36.094372 0
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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
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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

S131
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188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
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15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
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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


crystal
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216
5.62
2
13 0. 0. 0.
233 0.25 0.25 0.25
printout
basisset
end
end
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2.4904900 0.6125950 0.4491460
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0.1 1. 1.
0 1 3 3 1
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44.767415 198.307880 0

S134
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18.973471 56.871464 0
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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
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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
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3.20189 -0.320457
1.42096 -0.337391
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0.116735 0.534980
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0.321443 1
0 0 1 0 1
0.116735 1
0 2 7 6 1
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24.1195 -0.085101
5.84196 0.404762
2.56010 0.531478
1.09308 0.184012
0.318424 0.005764
0.100972 -0.00352
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2.56010 -0.172259
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0 3 7 10 1
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36.8872 0.079544
13.6893 0.236755
5.38964 0.401534
2.08046 0.406686
0.737568 0.173162
0.3078 0.008730
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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

Crystal

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216
5.448
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15 0.25 0.25 0.25

Printout

Basisset

End

231 9

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51.629117 -27.380273 0
15.241738 -1.587022 0
15.320193 -2.516292 0
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4.755103 0.202198 0
10.762263 -0.61699 0
19.852939 -3.138584 0
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420.664 0.002117
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2.67643 0.751559
1.13353 0.447202
0.207220 0.012746
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2848.20 -0.000097
420.664 -0.000614
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14.2207 0.126784
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0.1 1
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27.6822 0.085621
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248.7550000 0.3782090
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36.225700 0.627647
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0.1 1.000000
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end
ulhf
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
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216
6.1060
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252 0.25 0.25 0.25

Printout

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14.903524 46.057427 0
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43.698536 -20.543980 0
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12.228422 -1.062943 0
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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

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0.25082400e+01 0.14386170e+01
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0.15400200e+00 -0.11876310e+01
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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+00
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0.31687500e+01 -0.35121400e+00
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0.36664300e+00 0.57920500e+00
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0.36664300e+00 0.10000000e+01
252 6
input
6. 0 2 4 2 2 0

S142
B3PW
uhf
dft
biesplit
10
tolinteg
7 7 7 7 14
end
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
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end
FeO

FeO – Journal of Chemical Physics (1933) 1, p29-p36

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**Notes:**
- The numbers represent coefficients in a mathematical expression or equation.
- The format suggests this might be part of a larger dataset or table.
- The values are likely to be part of a numerical analysis or algebraic system.
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Crystal

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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
dend
uhf
dft
b3pw
dend
biesplit
10
tolinteg
7 7 7 7 14
sorestart
dend
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80

S163
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
0.0701
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 0.14836170e+01
0.10301900e+01 -0.98242900e+00
0.15400200e+00 -0.11876310e+01
0.010101
0.1 0.10000000e+01
0.2661
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
0.2601
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
0.2101
0.59572000e-01 0.10000000e+01
0.3661
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
0.36643000e+00 0.20225800e+00
0.3601
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
0.36643000e+00 0.57920500e+00
0.3101
0.36643000e+00 0.10000000e+01
2349
input
24.024620
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
0.0192 -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
0.210.1
0.1137 1
0.36 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
0.310.1
0.3656 1
99 0
end
uhf
dft
b3pw
end
biesplit
10
tolinteg
777714
end
12024
maxcycle
100
tolscf
77
fmixing
80
broyden
0.001
end
AgI


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

S169
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
S171
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
der
uhf
dft
b3pw
der
biesplit
10
tolinteg
7 7 7 7 14
der
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
der
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 0.3333333 0.6666667 0.3336
14 0.3333333 0.6666667 0.6671
6 0.3333333 0.6666667 0.4588
6 0.0 0.0 0.1254
6 0.3333333 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 1.00000000
6 5
0 0 6 2 1
4563.2400000 0.00196665
682.0240000 0.0152306

S174
S175
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
0.14518400e+00 0.15983000e+00
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
0.70973900e+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
0.12 0.10000000e+01
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
0.12 0.10000000e+01
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
0.12 0.10000000e+01
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
0.31 0.10000000e+01
0.28364200e+00 0.10000000e+01
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

S178
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 0.50811500e+00
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

S180
| 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 |
| 0.11054600e+02 0.21107100e+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+02 0.37537900e+00 |
| 0.18776000e+01 0.50840900e+00 |
| 0.79333500e+00 0.23909500e+00 |
| 0.19347600e+00 0.15850000e+1 |
| 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 0.51905000e+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 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

S182
0.19530100e+02  -0.18836000e-01
0.11088200e+02    0.80006000e-01
0.27156300e+01   -0.30665200e+00
0.12043000e+01   -0.14759400e+00
0.33995000e+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. 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

S184
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
TOLINTEGR
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


crystal

0 0 0
225
5.5463
2
247 0.00 0.00 0.00
17 0.5 0.5 0.5

printout
basisset
dend
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

S187
0.0701
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
0.14381400E+01 -0.12701730E+01
0.64838200E+00 0.53937300E+00
0.13588500E+00 0.16533910E+01
0.12 0.10000000E+01
0.2661
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
0.2601
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
0.2601
0.11875100E+02 -0.52857000E-01
0.80024500E+01 0.14703900E-01
0.20176600E+01 -0.31297300E+00
0.95423000E+00 -0.37082800E+00
0.42311800E+00 0.42362900E+00
0.13588500E+00 0.75365500E+00
0.2101
0.12 0.10000000E+01
0.3691
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
0.3601
0.26432000E+02 -0.47330000E-02
0.11034500E+02 0.19070000E+01
0.27378700E+01 -0.43329800E+00
0.11957500E+01 -0.44456800E+00

S188
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 0.3250200
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

S191
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

S193
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
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

S194
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
derivate
uhf
dft
b3pw
derivative
biesplit
10
tolinteg
7 7 7 7 14
derivative
12 0 24
maxcycle
100
tolscf
7 7
fmixing
80
broyden
0.0001
derivative
SrTiO₃


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
4.24198396 -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

S196
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
S197
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 0.684507810D-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
TiO$_2$ (Rutile)


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 0.2000190
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

S200
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
0.359993586D+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 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 0.66666667 0.00000
6 0.33333333 0.66666667 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 0.32502200
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 1.00000000
6 5
0 0 6 2 1
4563.2400000 0.00196665
682.0240000 0.0152306
154.9730000 0.0761269
44.4530000 0.2608010
13.0290000 0.6164620
1.8277300 0.2210060

S202
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

S204
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 0.50849000e+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 0.51905000e+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
105819.000000 0.0007380

S205
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)


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 0.684507810D-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
0.359993586D+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+00 .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
TOLINTEGR
7 7 7 7 14
MAXCYCLE
30
FMIXING
60
ANDERSON
PPAN
END
ZnO


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

S210
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


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 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
63.6016000 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

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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. 0. 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

S216
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

S217
30000000
MAXCYCLE
100
FMIXING
60
ANDERSON
PPAN
END
MgTe


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

S219
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
fmmixing
80
broyden
0.0001
end
ZnS


Crystal

0 0 0
2
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
39.886863 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
13961.700000 0.0057930
3169.910000 0.0299540
902.456000 0.1190280
297.158000 0.3684320
108.702000 0.5772990
  0 3 2 1
108.702000 0.1431860
43.1553000 0.6244650
18.1079000 0.2833660
  0 1 2 1
5.5600900 1.0000000
  0 1 0 1
2.1318300 1.0000000
  0 1 0 1
0.420430 1.0000000
  0 1 0 1
0.1360450 1.0000000
  0 2 4 6 1
495.040000 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

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
dend
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

S226
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 0.23995000e+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 0.51905000e+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 0.38147000e+00
0.28364200e+00 0.20062600e+00
0 3 6 0 1
0.60380400e+02 -0.22260000e-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

S228
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. 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 1.000000
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)


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 0.00145453 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
949.0400000 0.0149613
218.7760000 0.0735006
63.6916000 0.2489370
18.8282000 0.6024600

S234
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
0.6840000 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)


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
44.4530000 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
BIOPSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
END
**AlN (Wurtzite)**


**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 0.2468300
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


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

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
TOLINTEGR
7 7 7 9 30
TOLDEE
7
SHRINK
12 0 24
BIPOSIZE
30000000
EXCHSIZE
30000000
MAXCYCLE
50
FMIXING
60
ANDERSON
PPAN
NODIRECT
END

S243
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
38.7730000 0.3798170
0 0 3 2 1
38.7730000 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

S244
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 0.5814900
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$_2$ ($\beta$-cristobalite)


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
TOLINTEGR
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


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
8.6239000 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

S250
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

S251
SiO2 (α-quartz)


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 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 1.000000
0.12 1.000000
0.4500000 1.000000
5484.6717000 0.0018311
825.2349500 0.0139501
188.0469600 0.0684451
52.9645000 0.2327143
16.8975700 0.4701930
5.7996353 0.3585209
15.5396160 -0.1107775 0.0708743
3.5999336 -0.1480263 0.3397528
1.0137618 1.1307670 0.7271586
0.270058 1.0000000 1.000000
0.8 1.000000
99 0
END
DFT
B3PW
XLGRID
END
TOLINTEGR
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
1.875000 1.000000
0 3 1 0 1
0.187400 1.000000
0 3 1 0 1
4.912000 1.000000
0 4 1 0 1
0.182900 1.000000
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 1.000000
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