Supplementary Material for: [ Gaussian Basis sets for Crystalline Solids: All-Purpose Basis Set Libraries Vs System–Specific Optimizations]

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This document explicitly reports most of the CRYS\textsc{tal}17 inputs used to obtain the results reported in the paper. The basis set in the inputs are the dcm-XZVP obtained by using the BDIIS optimizer. The shells labelled by an asterisk are those that have been optimized.

1 Diamond - triple $\zeta$

\begin{verbatim}
DIAMOND-TZ-PBE
CRYSTAL
0 0 1
227
3.56679
1
6 0. 0. 0.
END
6 11
0 0 6 2. 1.
 1.35753496820E+04 2.22458143520E-04
 2.03523336800E+03 1.72327382520E-03
 4.63225623590E+02 8.92557153140E-03
 1.31200195980E+02 3.57279845020E-02
 4.28530158910E+01 1.10762599310E-01
 1.55841857660E+01 2.42956276260E-01
0 0 2 2. 1.
 6.20671385080E+00 4.14402634480E-01
 2.57648965270E+00 2.37449686550E-01
0 0 1 0. 1. *
 2.72877227664E+00 1.00000000000E+00
0 0 1 0. 1. *
 7.0825466129E-01 1.00000000000E+00
0 0 1 0. 1. *
 2.75435053993E-01 1.00000000000E+00
\end{verbatim}
0 2 4 2.1.
  3.46972322440E+01  5.3336578050E-03
  7.95826228260E+00  3.58641090920E-02
  2.3780268830E+00  1.42158733290E-01
  8.14332081830E-01  3.42704718450E-01
0 2 1 0.1. *
  6.18739070583E-01  1.00000000000E+00
0 2 1 0.1. *
  2.71282775658E-01  1.00000000000E+00
0 3 1 0.1. *
  2.0114380439E+00  1.00000000000E+00
0 3 1 0.1. *
  6.26539832528E-01  1.00000000000E+00
0 4 1 0.1. *
  1.06242225484E+00  1.00000000000E+00
99 0
END
DFT
PBE
END
MAXCYCLE
100
TOLINTEG
8 8 8 12 24
TOLDEE
8
SHRINK
8 8
END
Diamond - quadruple $\zeta$

DIAMOND-QZ-PBE

CRYSTAL

0 0 1
227
3.56679
1
6 0.0 0.
END

6 17
0 0 8 2.1.

6.70250710290E+04 3.87363085010E-05
1.00399865380E+04 3.01079175750E-04
2.28493169110E+03 1.57879180950E-03
6.47141221300E+02 6.60870871950E-03
2.11094723350E+02 2.33671232500E-02
7.61776438620E+01 7.04207168980E-02
2.96338391630E+01 1.73603449530E-01
1.21877850810E+01 3.22923056480E-01

0 0 2 2.1.

5.30260062990E+01 7.48974044920E-02
1.52585027760E+01 7.61362209830E-01

0 0 1 0.1.*

6.2060297512E+00 1.00000000000E+00
0 0 1 0.1.*

3.32497590179E+00 1.00000000000E+00
0 0 1 0.1.*

1.09521378286E+00 1.00000000000E+00
0 0 1 0.1.*

6.30358128105E-01 1.00000000000E+00
0 0 1 0.1.*

3.43646141101E-01 1.00000000000E+00
0 2 5 2. 1.
1.05125550820E+02 8.46475538440E-04
2.48844610660E+01 6.62740385340E-03
7.86372308260E+00 3.01203904190E-02
2.84070018350E+00 9.99514354760E-02
1.12271373350E+00 2.38262992820E-01
0 2 1 0. 1. *
8.74041963051E-01 1.00000000000E+00
0 2 1 0. 1. *
5.42561494412E-01 1.00000000000E+00
0 2 1 0. 1. *
1.83247854025E-01 1.00000000000E+00
0 3 1 0. 1. *
1.96394180988E+00 1.00000000000E+00
0 3 1 0. 1. *
9.68369087225E-01 1.00000000000E+00
0 3 1 0. 1. *
5.47772457307E-01 1.00000000000E+00
0 4 1 0. 1. *
1.51085897443E+00 1.00000000000E+00
0 4 1 0. 1. *
7.42254650983E-01 1.00000000000E+00
0 5 1 0. 1. *
1.18250314805E+00 1.00000000000E+00
99 0
END
DFT
PBE
END
MAXCYCLE
100
TOLINTEG
8 8 8 12 24
3 Graphene - triple $\zeta$

| GRAPHENE-TZ-PBE | SLAB | 77 | 2.47 | 1 | 6 | -0.33333333333 0.33333333333 0. |
|-----------------|------|----|------|---|---|----------------------------------|
| END             | 6    | 11 | 0    | 0 | 6 | 2. 1. |
|                 | 0.0  | 2.1. | 1.35753496820E+04 | 2.22458143520E-04 |
|                 | 0.0  | 2.1. | 2.03523336800E+03 | 1.72327382520E-03 |
|                 | 0.0  | 2.1. | 4.63225623590E+02 | 8.92557153140E-03 |
|                 | 0.0  | 2.1. | 1.31200195980E+02 | 3.57279845020E-02 |
|                 | 0.0  | 2.1. | 4.28530158910E+01 | 1.10762599310E-01 |
|                 | 0.0  | 2.1. | 1.55841857660E+01 | 2.42956276260E-01 |
|                 | 0.0  | 2.1. | 6.20671385080E+00 | 4.14402634480E-01 |
|                 | 0.0  | 2.1. | 2.57648965270E+00 | 2.37449686550E-01 |
|                 | 0.0  | 1. 0.1. * | 1.09605489209E+00 | 1.00000000000E+00 |
|                 | 0.0  | 1. 0.1. * | 5.91106934956E-01 | 1.00000000000E+00 |
0 0 1 0.1. *
  2.37383807053E-01  1.00000000000E+00
0 2 4 2.1.
  3.46972322440E+01  5.333336578050E-03
  7.95826228260E+00  3.58641090920E-02
  2.37808268830E+00  1.42158733290E-01
  8.14332081830E-01  3.42704718450E-01
0 2 1 0.1. *
  3.38693223652E-01  1.00000000000E+00
0 2 1 0.1. *
  1.59434147140E-01  1.00000000000E+00
0 3 1 0.1. *
  1.25021363036E+00  1.00000000000E+00
0 3 1 0.1. *
  7.19402508165E-01  1.00000000000E+00
0 4 1 0.1. *
  7.06699996366E-01  1.00000000000E+00
99 0
END
DFT
PBE
XLGRID
END
SCFDIR
FMIXING
30
LDREMO
1
MAXCYCLES
100
TOLINTEG
8 8 8 8 16
TOLDEE
4 Graphene - quadruple $\zeta$

```
GRAPHENE-QZ-PBE
SLAB
77
2.47
1
6 -0.33333333333 0.33333333333 0.
```

```
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 670250710290E+04 | 3.87363085010E-05 |
| 1.00399865380E+04 | 3.01079175750E-04 |
| 2.28493169110E+03 | 1.57879180950E-03 |
| 6.47141221300E+02 | 6.60870871950E-03 |
| 2.11094723350E+02 | 2.33671232500E-02 |
| 7.61776438620E+01 | 7.04207168980E-02 |
| 2.96338391630E+01 | 1.73603449530E-01 |
| 1.21877850810E+01 | 3.22923056480E-01 |
```

```
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 5.30260062990E+01 | 7.48974044920E-02 |
| 1.52585027760E+01 | 7.61362209830E-01 |
```

```
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 0 0 2 2.1 |
| 5.24039574640E+00 | 1.00000000000E+00 |
| 0 0 1 0.1.* |
```

```
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 2.32777405666E+00 | 1.00000000000E+00 |
| 0 0 1 0.1.* |
```
1.04613233770E+00 1.00000000000E+00
0 0 1 0.1. *
5.2183251512E-01 1.00000000000E+00
0 0 1 0.1. *
2.00431897163E-01 1.00000000000E+00
0 2 5 2.1.
1.05125550820E+02 8.46475538440E-04
2.4884610660E+01 6.62740385340E-03
7.86372308260E+00 3.01203904190E-02
2.84070018350E+00 9.99514354760E-02
1.1227137350E+00 2.38262992820E-01
0 2 1 0.1. *
4.50031980659E-01 1.00000000000E+00
0 2 1 0.1. *
3.28748485841E-01 1.00000000000E+00
0 2 1 0.1. *
1.24896018560E-01 1.00000000000E+00
0 3 1 0.1. *
1.91296701725E+00 1.00000000000E+00
0 3 1 0.1. *
8.63019243591E-01 1.00000000000E+00
0 3 1 0.1. *
4.52624895593E-01 1.00000000000E+00
0 4 1 0.1. *
1.41426143665E+00 1.00000000000E+00
0 4 1 0.1. *
5.9818943168E-01 1.00000000000E+00
0 5 1 0.1. *
9.93072428023E-01 1.00000000000E+00
99 0
END
DFT
DFT
PBE
5  Carbyne - triple ζ

C_Chain
POLYMER
1
2.56620186
2
6   9.624791798260E-02 -1.258372661974E-18 -4.072637834921E-09
6  -3.962479179826E-01 -2.785734209432E-16 4.072638114753E-09
END
6 11
0 0 6 2. 1.
1.35753496820E+04 2.22458143520E-04
2.03523336800E+03 1.72327382520E-03
4.63225623590E+02 8.92557153140E-03
LDREMO
1
SCFDIR
LEVSHIFT
10 1
FMIXING
30
MAXCYCLES
100
TOLINTEG
8 8 8 8 16
TOLDEE
8
SHRINK
64 64
END

6   NaCl - triple $\zeta$

NaCl_crystal-TZ-PBEO
CRYSTAL
0 0 0
225
5.6402
2
17 0.0 0.0 0.0
11 0.5 0.5 0.5
END

11 11
0 0 7 2.1.

2.60411099270E+04  6.18063428110E-04
3.90612685480E+03  4.77486044140E-03
| x       | y       | z       | dx      | dy      | dz      |
|---------|---------|---------|---------|---------|---------|
| 8.8974549930E+02 | 2.44716848290E-02 |
| 2.51454979610E+02 | 9.4753949770E-02 |
| 8.16501435120E+01 | 2.68674969200E-01 |
| 2.89041584010E+01 | 4.79254754400E-01 |
| 1.06257829320E+01 | 3.32485914690E-01 |
| 0 0 3 2.1. | 5.37694101790E+01 | 1.95277318720E-02 |
| 1.63082430250E+01 | 9.26480107940E-02 |
| 2.37303841250E+00 | -3.99386701720E-01 |
| 0 0 2 1.1. | 9.57307726030E-01 | 1.64285953910E+00 |
| 4.08064609590E-01 | 5.5692596660E-01 |
| 0 0 1 0.1.* | 3.43569978393E-01 | 9.99992062637E-01 |
| 0 0 1 0.1.* | 8.28104267544E-02 | 9.99700925116E-01 |
| 0 2 5 6.1. | 1.38079799890E+02 | 5.79518919290E-03 |
| 3.22327003930E+01 | 4.16208462510E-02 |
| 9.98160753600E+00 | 1.62819168850E-01 |
| 3.48220339280E+00 | 3.6011784670E-01 |
| 1.22991346200E+00 | 4.4858979890E-01 |
| 0 2 1 0.1.* | 4.02257637589E-01 | 1.00001437874E+00 |
| 0 2 1 0.1.* | 9.81092534535E-02 | 1.000010780928E+00 |
| 0 3 1 0.1.* | 2.60738659094E+00 | 1.00000000000E+00 |
| 0 3 1 0.1.* | 4.03951011422E-01 | 1.00000000000E+00 |
| 0 3 1 0.1.* | 9.84682729829E-02 | 1.00000000000E+00 |
| 17 13 |
0 0 7 2.1.
6.95079909450E+04 5.43148974970E-04
1.04261568800E+04 4.19904639610E-03
2.37323406100E+03 2.15921416790E-02
6.71564200710E+02 8.45988500940E-02
2.18419997900E+02 2.47572497240E-01
7.75724971400E+01 4.70169302280E-01
2.88881527700E+01 3.74363707160E-01

0 0 3 2.1.
1.27105271850E+02 2.51821666030E-02
3.93395829610E+01 1.07861124560E-01
7.67406799890E+00 -2.74088215740E-01

0 0 2 2.1.
3.87456276300E+00 1.32138750140E+00
1.83858325730E+00 6.86369536800E-01

0 0 1 0.1 *
5.72362924707E-01 1.00000000308E+00

0 0 1 0.1 *
2.31162823985E-01 9.99999997835E-01

0 2 5 6.1.
6.66504232840E+02 2.36326638360E-03
1.57642416900E+02 1.88793003740E-02
5.02625209780E+01 8.72063412730E-02
1.85360781050E+01 2.52856129700E-01
7.29405327770E+00 4.35071548200E-01

0 2 1 5.1 *
2.93863280310E+00 1.00000000143E+00

0 2 1 0.1 *
1.19026410565E+00 1.00000000000E+00

0 2 1 0.1 *
4.69704038156E-01 1.00000000000E+00

0 2 1 0.1 *
1.74720163208E-01 1.00000000000E+00
0 3 2 0. 1.
  4.61000000000E+00  2.00000000000E-01
  1.01100000000E+00  1.00000000000E+00
0 3 1 0. 1. *
  2.83798017576E-01  1.00000000000E+00
0 4 1 0. 1. *
  6.89848600893E-01  1.00000000000E+00
99 0
END
DFT
PBE0
END
TOLINTEG
8 8 8 8 16
TOLDEE
8
SHRINK
8 8
END

7 Na - triple ζ

Na_crystal-TZ-PBE0
CRYSTAL
0 0 0
229
4.2906
1
11 0. 0. 0.
END
11 11
0 0 7 2. 1.
2.60411099270E+04  6.18063428110E-04
3.90612685480E+03  4.77486044140E-03
8.88974549930E+02  2.44716848290E-02
2.51454979610E+02  9.47553949770E-02
8.16501435120E+02  3.32485914690E-01
2.89041584010E+01  4.79254754400E-01
1.06257829320E+01  3.32485914690E-01
0 0 3 2.1.
5.37694101790E+01  1.95277318720E-02
1.63082430250E+01  9.26480107940E-02
2.37303841250E+00  -3.99386701720E-01
9.57307726030E-01  5.56925966600E-01
0 0 1 0.1. *
2.12721167582E-01  9.9999262637E-01
0 0 1 0.1. *
7.82096876345E-02  9.99700925116E-01
0 2 5 6.1.
1.38079799890E+02  5.79518919290E-03
3.22327003930E+01  4.16208462510E-02
9.98160753600E+00  1.6281968850E-01
3.48220339280E+00  3.60117846470E-01
1.22991346200E+00  4.48589798890E-01
0 2 1 0.1. *
4.03415531731E-01  1.00001437874E+00
0 2 1 0.1. *
8.50539333916E-02  1.00010780928E+00
0 3 1 0.1. *
2.60862497919E+00  1.00000000000E+00
0 3 1 0.1. *
4.33739110192E-01  1.00000000000E+00
0 3 1 0.1. *
1.11542851169E-01  1.00000000000E+00
99  0
END
DFT
PBE0
END
TOLINTEG
8 8 8 8 16
TOLDEE
8
SHRINK
8 8
END

8  Cl$_2$ - triple $\zeta$

Cl$_\text{crystal-TZ-PBE0}$

CRYSTAL
0 0 0
64
7.77875  4.34941  9.02754
8
17  0  0.40882  0.89848
17  0  0.09118  0.39848
17  0  0.90882  0.60152
17  0  0.59118  0.10152
17  0.50000  0.90882  0.89848
17  0.50000  0.59118  0.39848
17  0.50000  0.40882  0.60152
17  0.50000  0.09118  0.10152
END
17  13
9  LiH - SVP

LiH-SVP-HF
CRYSTAL
0 0 0
225
4.084
2
3 0.0 0.0 0.0
1 0.5 0.5 0.5
END

19
0 0 5 2.1.
 2.66277855160E+02 6.49201503250E-03
 4.00697834470E+01 4.77478632150E-02
 9.0599443890E+00 2.02687961110E-01
 2.4503090510E+00 4.86065748170E-01
 7.22095718550E-01 4.36269779550E-01
0 0 1 1.1. *
 9.22176144583E-01 1.00000000000E+00
0 0 1 0.1. *
 3.26710606911E-01 1.00000000000E+00
0 2 2 0.1.
 1.45000000000E+00 2.58600000000E-01
 3.00000000000E-01 1.00000000000E+00
0 2 1 0.1. *
 2.44108651001E-01 1.00000000000E+00
1 3
0 0 3 1.1.
 1.30107010000E+01 1.96821580000E-02
 1.96225720000E+01 1.37965240000E-01
 4.44537960000E-01 4.78319350000E-01
0 0 1 0.1. *
 1.12026126213E-01 1.00000000000E+00
0 2 1 0.1. *
 7.04259338539E-01 1.00000000000E+00
99 0
END
TOLINTEG
8 8 8 15 30
SHRINK
8 8
FMIXING
50
TOLDEE
10 LiH - triple $\zeta$

LiH-TZ-HF
CRYSTAL
0 0 0
225
4.084
2
3 0.0 0.0 0.0
1 0.5 0.5 0.5
END

3 8
0 0 6 2.1.
  6.26926280100E+03  2.05409688260E-04
  9.40316124310E+02  1.59165540890E-03
  2.14221075280E+02  8.28698297070E-03
  6.07598401840E+01  3.38563742490E-02
  1.99151520320E+01  1.11032258760E-01
  7.31715097970E+00  2.7449383390E-01

0 0 2 1.1.
  2.97246742160E+00  2.37924564110E-01
  1.26398523140E+00  3.07654119240E-01

0 0 1 0.1. *
  7.80051836987E-01  1.00000000000E+00

0 0 1 0.1. *
  3.56751423380E-01  1.00000000000E+00

0 0 1 0.1. *
  1.32441081592E-01  1.00000000000E+00

0 2 1 0.1. *
11 **LiH - quadruple $\zeta$**

LiH-QZ-HF
CRYSTAL
0 0 0
225
4.084
2
3 0.0 0.0 0.0
1 0.5 0.5 0.5
LATVEC
100000
END

1 10

0 0 4 1.1.
1.90691690000E+02 7.08151670000E-04
2.86055320000E+01 5.46788270000E-03
6.50959430000E+00 2.79660500000E-02
1.84124550000E+00 1.07645380000E-01
0 0 1 0.1.*
6.39685855118E-01 1.00000000000E+00
0 0 1 0.1.*
2.72584652976E-01 1.00000000000E+00
0 0 1 0.1.*
1.44295727123E-01 1.00000000000E+00
0 2 1 0.1.*
2.29203807546E+00 1.00000000000E+00
0 2 1 0.1.*
8.3796510305E-01 1.00000000000E+00
0 2 1 0.1.*
2.95979305342E-01 1.00000000000E+00
0 3 1 0.1.*
2.06195543104E+00 1.00000000000E+00
0 3 1 0.1.*
6.61486854173E-01 1.00000000000E+00
0 4 1 0.1.*
1.39686108048E+00 1.00000000000E+00
3 13
0 0 9 2. 1.
  1.48539770850E+04  4.27113888150E-05
  2.22522364770E+03  3.32353108000E-04
  5.04873900800E+02  1.75184364900E-03
  1.42458475480E+02  7.34779958500E-03
  4.63155995800E+01  2.58983768300E-02
  1.66553354700E+01  7.66706824310E-02
  6.43311861990E+00  1.82760757650E-01
  2.60270438580E+00  3.26554340380E-01
  1.08972454050E+00  3.70004298280E-01
0 0 2 1. 1.
  4.42365959710E+00  1.11209879210E-01
  1.23663949900E+00  7.99873358620E-01
0 0 1 0. 1. *
  1.47258539716E+00  1.00000000000E+00
0 0 1 0. 1. *
  9.61687138188E-01  1.00000000000E+00
0 0 1 0. 1. *
  5.44705804681E-01  1.00000000000E+00
0 0 1 0. 1. *
  2.5977525362E-01  1.00000000000E+00
0 2 3 0. 1.
  3.26051092060E+00  8.65047902300E-03
  6.50030431150E-01  4.76141237360E-02
  1.69416710730E-01  2.10011380000E-01
0 2 1 0. 1. *
  3.83906409071E-01  1.00000000000E+00
0 2 1 0. 1. *
  1.98706020944E-01  1.00000000000E+00
0 2 1 0. 1. *
  3.72683460316E+00  1.00000000000E+00
0 3 1 0. 1. *
   3.33113752884E-01  1.00000000000E+00
0 3 1 0. 1. *
   3.68482801264E-01  1.00000000000E+00
0 4 1 0. 1. *
   1.75294244744E-01  1.00000000000E+00
99 0
END
TOLINTEG
10 10 10 40 160
SHRINK
12 12
NOBIPOLA
LDREMO
1
FMIXING
96
THREDIIS
2
TOLDEE
10
ILASIZE
20000
END