Range-separated double-hybrid density-functional theory applied to periodic systems

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Supplementary Material

The original cc-pVQZ for Lithium was re-optimized (exponents of the outermost s and p Gaussian functions and polarization functions) for solid state calculations of LiH bulk at the HF level of theory in combination with a cc-pVQZ basis set for Hydrogen. The same basis set has been used by some of us in a previous work[1].
The basis set is reported in the Table I below in the CRYSTAL format.

By starting from the original cc-pVDZ basis set for Silicon, the exponents of the uncontracted s and p Gaussian functions were tuned by applying the same scaling factor. The exponent of the polarizazion function was optimized as well.
The input of modified cc-pVDZ basis set for Silicon is reported in Table II.

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[1] D. Usvyat, B. Civalleri, L. Maschio, R. Dovesi, C. Pisani, and M. Schütz, J. Comp. Phys. **134**, 214105 (2011).

3 10	
0 0 9 2. 1.	
6.601E+03	1.170E-04
9.897E+02	9.110E-04
2.257E+02	4.728E-03
6.429E+01	1.920E-02
2.118E+01	6.305E-02
7.724E+00	1.632E-01
3.003E+00	3.148E-01
1.212E+00	3.939E-01
4.930E-01	1.969E-01
0 0 9 2. 1.	
6.601E+03	-1.800E-05
9.897E+02	-1.420E-04
2.257E+02	-7.410E-04
6.429E+01	-3.020E-03
2.118E+01	-1.012E-02
7.724E+00	-2.709E-02
3.003E+00	-5.736E-02
1.212E+00	-9.390E-02
4.930E-01	-1.211E-01
0 0 1 0. 1.	
5.700E-01	1.000E+00
0 0 1 0. 1.	
2.100E-01	1.000E+00
0 2 3 0. 1.	
6.250E+00	3.388E-03
1.370E+00	1.932E-02
3.672E-01	7.910E-02
0 2 1 0. 1.	
9.500E-01	1.000E+00
0 2 1 0. 1.	
2.200E-01	1.000E+00
0 3 1 0. 1.	
1.800E+00	1.000E+00
0 3 1 0. 1.	
6.000E-01	1.000E+00
0 4 1 0. 1.	
7.000E-01	1.000E+00

Table I: Basis set for Lithium used for calculation on LiH and LiF

14 8	
0 0 11 2. 1.	
7.886E+04	2.704E-04
1.182E+04	2.097E-03
2.692E+03	1.085E-02
7.634E+02	4.368E-02
2.496E+02	1.377E-01
9.028E+01	3.166E-01
3.529E+01	4.186E-01
1.451E+01	2.102E-01
4.053E+00	1.450E-02
1.482E+00	-2.036E-03
2.517E-01	6.242E-04
0 0 11 2. 1.	
7.886E+04	-7.232E-05
1.182E+04	-5.551E-04
2.692E+03	-2.938E-03
7.634E+02	-1.177E-02
2.496E+02	-4.029E-02
9.028E+01	-1.006E-01
3.529E+01	-1.965E-01
1.451E+01	-1.024E-01
4.053E+00	5.272E-01
1.482E+00	5.933E-01
2.517E-01	3.327E-02
0 0 11 2. 1.	
7.886E+04	1.851E-05
1.182E+04	1.422E-04
2.692E+03	7.522E-04
7.634E+02	3.023E-03
2.496E+02	1.037E-02
9.028E+01	2.626E-02
3.529E+01	5.240E-02
1.451E+01	2.910E-02
4.053E+00	-1.780E-01
1.482E+00	-3.469E-01
2.517E-01	6.230E-01
0 0 1 0. 1.	
1.118E-01	1.000E+00
0 2 7 6. 1.	
3.159E+02	3.927E-03
7.442E+01	2.988E-02
2.348E+01	1.272E-01
8.488E+00	3.209E-01
3.217E+00	4.554E-01
1.229E+00	2.686E-01
2.964E-01	1.883E-02
0 2 7 2. 1.	
3.159E+02	-8.583E-04
7.442E+01	-6.303E-03
2.348E+01	-2.883E-02
8.488E+00	-6.946E-02
3.217E+00	-1.195E-01
1.229E+00	-1.996E-02
2.964E-01	5.103E-01
0 2 1 0. 1.	
1.061E-01	1.000E+00
0 3 1 0. 1.	
4.297E-01	1.000E+00

Table II: Modified cc-pVDZ basis set for Silicon.