

Supplementary Materials: A Visual Representation for Accurate Local Basis Set Construction and Optimization: A Case Study of SrTiO₃ with Hybrid DFT Functionals

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Table S1. Four basis sets (BSs) as used in the present study for SrTiO₃.

Sr	Ti	O
	BS1 (developed in this work)	
38 17	22 14	8 9
0 0 12 2 1	0 0 12 2 1	0 0 9 2 1
1.3008E+07 1.7112E-05	2.9508E+06 2.5773E-05	6.8509E+04 1.8658E-04
1.9480E+06 1.3317E-04	4.4309E+05 1.9954E-04	1.0260E+04 1.4609E-03
4.4315E+05 7.0355E-04	1.0068E+05 1.0567E-03	2.3368E+03 7.5824E-03
1.2531E+05 2.9642E-03	2.8486E+04 4.4448E-03	6.6273E+02 3.1661E-02
4.0842E+04 1.0816E-02	9.2830E+03 1.6134E-02	2.1610E+02 1.0957E-01
1.4722E+04 3.4975E-02	3.3482E+03 5.1880E-02	7.7886E+01 3.1065E-01
5.7284E+03 1.0186E-01	1.3069E+03 1.4646E-01	3.0725E+01 6.5334E-01
2.3651E+03 2.6496E-01	5.3962E+02 3.6988E-01	1.2559E+01 1.0000E+00
1.0325E+03 5.6546E-01	2.3210E+02 7.2964E-01	5.0498E+00 6.3468E-01
4.6955E+02 9.8241E-01	1.0625E+02 1.0000E+00	0 0 5 2 1
2.1830E+02 1.0000E+00	4.8974E+01 7.6151E-01	7.7886E+01 -1.3985E-02
1.0446E+02 4.9604E-01	2.1772E+01 1.6551E-01	3.0725E+01 -4.2044E-02
0 0 9 2 1	0 0 8 2 1	1.2559E+01 -2.3586E-01
5.7284E+03 -3.4538E-04	1.3069E+03 -8.6117E-04	5.0498E+00 -3.7112E-01
2.3651E+03 -3.3609E-03	5.3962E+02 -6.2440E-03	1.6519E+00 1.0000E+00
1.0325E+03 -1.6183E-02	2.3210E+02 -2.7195E-02	0 0 1 0 1
4.6955E+02 -6.7820E-02	1.0625E+02 -1.0042E-01	6.5218E-01 1.0000E+00
2.1830E+02 -1.7954E-01	4.8974E+01 -1.6690E-01	0 0 1 0 1
1.0446E+02 -7.9275E-02	2.1772E+01 1.5170E-01	2.3319E-01 1.0000E+00
4.4473E+01 7.3069E-01	9.7296E+00 1.0000E+00	0 2 4 6 1
2.1749E+01 1.0000E+00	4.4200E+00 8.0444E-01	1.6529E+02 7.8933E-03
1.0910E+01 3.7270E-01	0 0 3 2 1	3.5729E+01 7.6559E-02
0 0 4 2 1	9.7296E+00 -2.7097E-01	1.1128E+01 3.2279E-01
4.4473E+01 -5.5340E-02	4.4200E+00 -7.3938E-01	3.9311E+00 1.0000E+00
2.1749E+01 -3.4720E-01	1.8970E+00 1.0000E+00	0 2 1 0 1
1.0910E+01 2.7192E-02	0 0 1 0 1	1.4955E+00 1.0000E+00
4.8719E+00 1.0000E+00	8.1421E-01 1.0000E+00	0 2 1 0 1
0 0 1 0 1	0 0 1 0 1	5.4262E-01 1.0000E+00
2.3675E+00 1.0000E+00	3.2437E-01 1.0000E+00	0 2 1 0 1
0 0 1 0 1	0 2 7 6 1	1.6891E-01 1.0000E+00
9.6120E-01 1.0000E+00	2.3471E+03 1.7410E-03	0 3 1 0 1
0 0 1 2 1	5.4908E+02 1.5049E-02	7.6783E-01 1.0000E+00
4.6525E-01 1.0000E+00	1.8090E+02 7.4700E-02	
0 0 1 0 1	6.9228E+01 2.5919E-01	
1.9854E-01 1.0000E+00	2.8803E+01 6.4419E-01	
0 2 9 6 1	1.2347E+01 1.0000E+00	
2.0566E+04 3.4021E-04	5.4678E+00 6.6348E-01	
4.8545E+03 3.0402E-03	0 2 5 6 1	
1.5324E+03 1.8509E-02	6.9228E+01 -3.6627E-03	

5.7714E+02 7.8057E-02	2.8803E+01 -2.6575E-02
2.4504E+02 2.4422E-01	1.2347E+01 -5.5743E-02
1.1197E+02 5.9143E-01	5.4678E+00 3.7059E-02
5.2273E+01 1.0000E+00	2.3662E+00 1.0000E+00
2.4946E+01 8.4150E-01	0 2 1 0 1
1.2023E+01 2.7033E-01	1.0065E+00 1.0000E+00
0 2 7 6 1	0 2 1 0 1
2.4504E+02 -2.8573E-03	4.0462E-01 1.0000E+00
1.1197E+02 -1.7097E-02	0 3 5 0 1
5.2273E+01 -4.5177E-02	2.4906E+02 1.3058E-03
2.4946E+01 -1.0086E-02	6.8579E+01 1.6566E-02
1.2023E+01 4.6393E-01	2.3943E+01 9.3467E-02
5.6544E+00 1.0000E+00	9.6662E+00 3.4426E-01
2.7104E+00 6.9897E-01	3.8247E+00 1.0000E+00
0 2 5 6 1	0 3 1 0 1
2.4946E+01 -4.2362E-04	1.5087E+00 1.0000E+00
1.2023E+01 -2.2829E-02	0 3 1 0 1
5.6544E+00 -8.3487E-02	5.5267E-01 1.0000E+00
2.7104E+00 -1.0298E-01	0 3 1 0 1
1.2092E+00 1.0000E+00	2.5572E-01 1.0000E+00
0 2 1 0 1	0 4 1 0 1
5.4011E-01 1.0000E+00	4.9341E-01 1.0000E+00
0 2 1 0 1	
2.1179E-01 1.0000E+00	
0 3 7 10 1	
9.1733E+02 1.1361E-03	
2.7400E+02 1.0727E-02	
1.0576E+02 5.7934E-02	
4.5627E+01 2.2058E-01	
2.0539E+01 5.5343E-01	
9.7749E+00 9.0596E-01	
4.6411E+00 1.0000E+00	
0 3 1 0 1	
2.1186E+00 1.0000E+00	
0 3 1 0 1	
9.1489E-01 1.0000E+00	
0 3 1 0 1	
3.0031E-01 1.0000E+00	
0 4 1 0 1	
5.1862E-01 1.0000E+00	

BS2 ^a

238 7	222 16	8 5
INPUT	INPUT	0 0 6 2 1
10 5 7 7 7 0 0	12 4 6 6 0 0 0	8588.5 0.00189515
2.23399997 -1.16187501 0	8.02050018 -2.92140889 0	1297.23 0.0143859
5.671 -13.3739996 0	23.73159981 -21.51072121 0	299.296 0.070732
13.8817997 -43.23659134 0	76.42070007 -53.50305176 0	87.3771 0.240001
44.81060028 -100.0990372 0	255.1517944 -8.1329937 -1	25.6789 0.594797
132.9026032 -20.51813126 -1	2.09669995 -51.37191772 0	3.74004 0.280802
2.4467001 53.58986664 0	2.54419994 113.3274994 0	0 1 3 6 1
2.8678 -172.0821838 0	3.42569995 -173.0386658 0	42.1175 0.113889 0.0365114
3.86610007 345.5859375 0	4.62150002 146.5667267 0	9.62837 0.920811 0.237153
5.66069984 -351.2217102 0	1.50059998 6.99775124 -1	2.85332 -0.00327447 0.819702
8.30790043 257.342865 0	18.84980011 3.13227606 -2	0 1 1 0 1

23.4951992 12.91709232 -1	3.53789997 32.56519318 0	0.878473787 1 1
21.03380013 6.33449411 -2	4.22800016 -122.7730484 0	0 1 1 0 1
2.20950007 49.15122604 0	5.74259996 217.986908 0	0.228702942 1 1
2.58439994 -158.8258209 0	7.77629995 -168.7288208 0	0 3 1 0 1
3.4684 320.0846252 0	11.05430031 5.54500103 -1	0.148050011 1
5.06430006 -349.1076965 0	3.2657001 4.74136782 -2	
7.37960005 239.3299103 0	0 0 1 2 1	
22.22710037 11.86419868 -1	39.81 1	
19.91810036 5.33859777 -2	0 0 1 2 1	
1.4073 32.67572403 0	12.22 1	
1.62419999 -103.2213364 0	0 0 1 0 1	
2.11750007 193.2765045 0	5.009 1	
2.97239995 -248.6330261 0	0 0 1 0 1	
4.11800003 183.3956604 0	1.286 1	
12.52390003 10.14631939 -1	0 0 1 0 1	
10.88269997 7.38135815 -2	0.614879662 1	
0 0 1 2 1	0 2 1 6 1	
1.553 1	36.37 1	
0 0 1 2 1	0 2 1 0 1	
1.071 1	14.78 1	
0 0 1 0 1	0 2 1 0 1	
0.345157821 1	6.275 1	
0 2 1 6 1	0 2 1 0 1	
3.004 1	2.479 1	
0 2 1 0 1	0 2 1 0 1	
0.729621681 1	1.016 1	
0 2 1 0 1	0 2 1 0 1	
0.275696365 1	0.3425734 1	
0 3 1 0 1	0 3 1 2 1	
0.502936699 1	25.99 1	
	0 3 1 0 1	
	7.086 1	
	0 3 1 0 1	
	2.349 1	
	0 3 1 0 1	
	0.73987416 1	
	0 3 1 0 1	
	0.293612329 1	

BS3^b

Sr_HAYWSC-311(1d)G_Piskunov_2004	Ti_HAYWSC-411(311d)G_Piskunov_2004	O_8-411d1_Bredow_2006 ^c
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BS4^d

Sr_POB-TZVP-rev2	Ti_POB-TZVP-rev2	O_POB-TZVP-rev2
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^a Introduced in Ref. [1]. ^b Introduced in Ref. [2] and given in CRYSTAL basis sets library Ref. [3] with the corresponding notation. ^c The oxygen basis set O_8-411d1-Bredow_2006 in [3] is firstly used in Ref. [2]. ^d Introduced in Refs. [4,5] and given in CRYSTAL basis sets library Ref. [3] with the corresponding notation.

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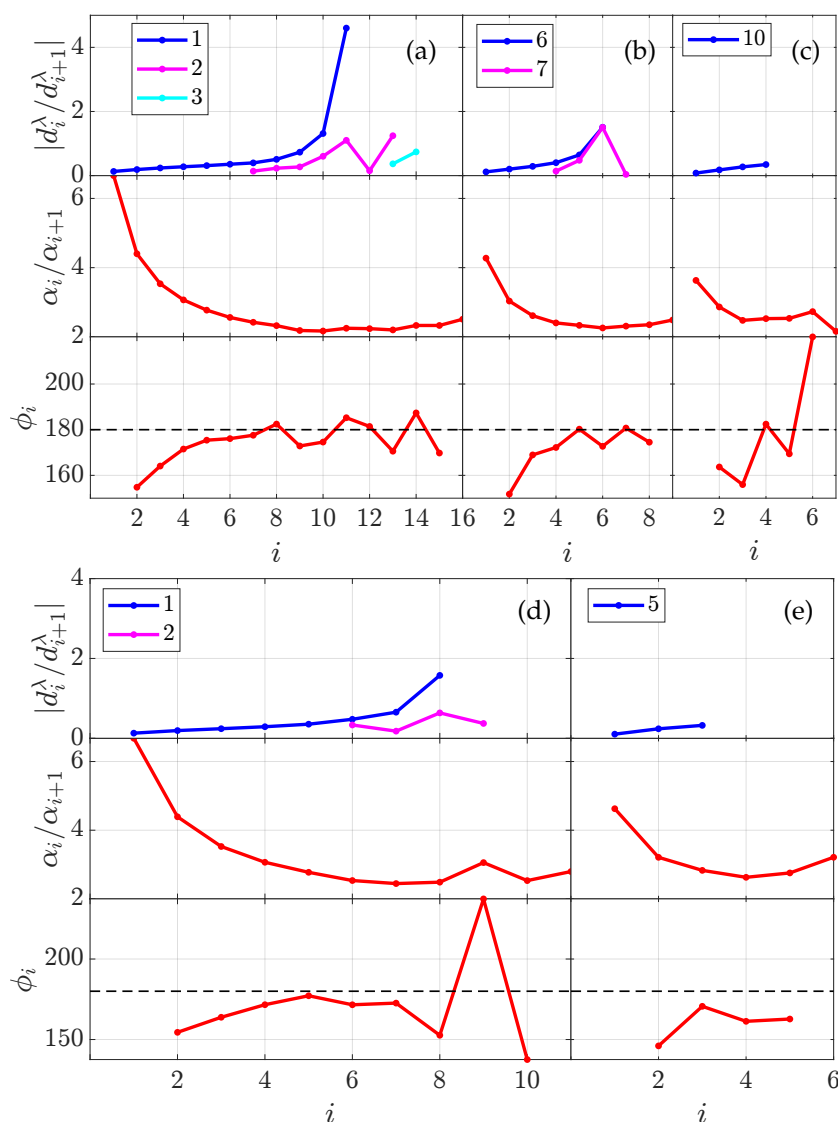


Figure S1. Visual representation of Ti: (a) *s*-type, (b) *p*-type, and (c) *d*-type and O: (d) *s*-type and (e) *p*-type basis coefficients from BS1 (Table S1): modulus of consecutive contraction coefficients $|d_i^\lambda / d_{i+1}^\lambda|$, where shell index, λ , is provided in the legend, the ratio of successive nonredundant exponents, α_i / α_{i+1} , and angle, ϕ_i , between ratios $(\alpha_{i-1} / \alpha_i, \alpha_i / \alpha_{i+1}, \alpha_{i+1} / \alpha_{i+2})$. The dashed line denotes $\phi_i = 180^\circ$.

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