Computational Procedure to an accurate DFT simulation to solid state systems

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Supplementary information

Table S1 - Optimized lattice parameters (Å) and band gap energy (E_{gap}, eV) of *$BaMoO_4$*. The differences (%) from the experimental values are shown in parentheses.

Functional	*a=b*	*c*	E_{gap}
B1WC	5.53 (-0.90)	12.57 (-1.95)	5.05 (+11.23)
B3PW	5.59 (+0.18)	12.76 (-0.46)	5.41 (-19.16)
PBE0	5.58 (0.00)	12.71 (-0.85)	5.87 (+29.30)
PBESOL0	5.53 (-0.90)	12.54 (-2.18)	5.93 (+30.61)
SOGGAXC	5.51 (-1.25)	12.63 (-1.48)	3.66 (-19.38)
HSE06	5.58 (0.00)	12.71 (-0.85)	5.13 (+13.00)
WC1LYP	**5.56 (-0.35)**	**12.75 (-0.54)**	**4.98 (+9.70)**
B3LYP	5.62 (+0.71)	12.87 (-0.23)	5.35 (+17.84)
Experimental[39]	5.58	12.82	4.54

Table S2 – HF percentage analysis of the hybrid functionals using the optimized atomic basis set (BasisOpt/HF%). The lattice parameters (Å), band gap energy (E_{gap}, eV) and the differences (%) from the experimental values are shown in parentheses.

	WC1LYP			**B3LYP**		
HF %	***a***	***c***	E_{gap}	***a***	***c***	E_{gap}
3%	5.63 (+0.89)	12.82 (0.00)	3.66 (-19.38)	5.68 (+1.80)	13.03 (+1.63)	3.68 (-18.94)
6%	5.63 (+0.89)	12.80 (-0.15)	3.92 (-13.65)	5.68 (+1.80)	13.01 (+1.48)	3.94 (-13.21)
10%	5.63 (+0.89)	12.78 (-0.31)	4.27 (-5.95)	5.68 (+ 1.80)	12.98 (+1.25)	4.29 (-5.51)
12%	**5.63 (+0.89)**	**12.77 (-0.39)**	**4.45 (-1.98)**	**5.68 (+1.80)**	**12.97 (+1.17)**	**4.48 (-1.32)**
14%	5.68 (+1.80)	12.98 (+1.24)	4.65 (+2.42)	5.68 (+1.80)	12.96 (+1.09)	4.65 (+2.42)

Table S3 – HF exchange percentage analysis of the hybrid functionals of the original atomic basis (HF%/BasisOpt) The lattice parameters (Å), band gap energy (E_{gap}, eV) and the differences (%) from the experimental values are shown in parentheses.

	WC1LYP			**B3LYP**		
HF%	***a***	***c***	E_{gap}	***a***	***c***	E_{gap}
3%	5.56 (-0.35)	12.79 (-0.23)	3.81 (-16.08)	5.62 (+0.71)	12.96 (+1.09)	3.8 (-16.30)
6%	5.56 (-0.35)	12.78 (-0.31)	4.08 (-10.13)	5.62 (+0.71)	12.95 (+1.01)	4.06 (-10.57)
10%	5.56 (-0.35)	12.76 (-0.46)	4.44 (-2.20)	5.62 (+0.71)	12.92 (+0.78)	4.42 (-2.64)
12%	**5.56 (-0.35)**	**12.75 (-0.54)**	**4.62 (+1.76)**	**5.62 (+0.71)**	**12.91 (+0.70)**	**4.61 (+1.54)**
14%	5.57 (-0.17)	12.74 (-0.62)	4.8 (+5.72)	5.62 (+0.71)	12.90 (+0.62)	4.79 (+5.50)

The original basis set are shown on the following pages and the position of each optimized exponents for substitution are highlighted in red.

Barium Basis set

56 10

0 0 9 2.0 1.0

5268534.5 0.0000487

770380.75 0.000399

165754.0 0.00231

43022.7 0.0111

12502.388 0.046

3992.6684 0.1534

1421.8082 0.3477

567.1226 0.433

238.96431 0.2053

0 1 7 8.0 1.0

15454.316 -0.000378 0.0011

3602.2466 -0.00636 0.00992

1118.05623 -0.0517 0.0574

403.42504 -0.1463 0.2166

165.63812 0.0839 0.4578

77.56938 0.6077 0.4717

38.15578 0.5106 0.2341

0 1 6 8.0 1.0

387.66574 0.00625 -0.0124

146.12605 -0.0215 -0.0742

59.60664 -0.3106 -0.00329

27.24022 -0.0856 0.8572

13.08315 0.9117 1.3915

6.49829 0.554 0.5311

0 3 6 10.0 1.0

436.904 0.0151

130.498 0.1041

49.0975 0.3255

20.5988 0.4708

9.4682 0.2707

4.5895 0.0473

0 1 3 8.0 1.0

9.9542 0.5334 -0.1412

6.4094 0.1985 0.2844

3.2089 0.0769 0.2868

0 3 3 10.0 1.0

8.4525 0.2177

3.4646 0.5783

1.4564 0.4139

0 3 1 0.0 1.0

0.4539 ($^{1}\alpha_{sp}$) 1.0

0 1 3 8.0 1.0

5.1897 0.1986 0.2803

2.4353 0.959 1.3841

1.173 0.4417 0.6019

0 1 1 2.0 1.0

0.572 (α_{d}) 1.0 1.0

0 1 1 0.0 1.

0.5286 ($^{2}\alpha_{sp}$) 1.0 1.0

Molibdenium Basis set

42 9

0 0 9 2.0 1.0

2803592.825747 0.00005

444817.867538 0.000355

97623.996506 0.00215

24043.681147 0.0112

6747.518431 0.0473

2131.383958 0.1567

752.716925 0.3532

293.984852 0.4244

120.908020 0.1667

0 1 7 8.0 1.0

8300.696289 -0.000336 0.001

1904.293335 -0.00655 0.00936

572.519470 -0.0576 0.0567

198.596466 -0.1475 0.2205

77.368034 0.2011 0.4589

33.814167 0.6759 0.4095

15.491380 0.3038 0.1253

0 1 6 8.0 1.0

180.935425 0.00529 -0.0139

66.122765 -0.0394 -0.0723

27.487516 -0.3338 0.0737

11.638353 0.1347 0.9517

5.152159 0.9806 1.2527

2.264732 0.2897 0.3209

0 3 6 10.0 1.0

293.95 0.00793

87.2824 0.0589

32.1457 0.218

12.9741 0.4242

5.3868 0.4127

2.211 0.1305

0 1 3 8.0 1.0

4.4173 -2.8714 -0.0766

1.9173 0.2991 0.52

0.8516 7.9229 1.0991

0 1 1 0.0 1.0

0.3534 ($^{1}\alpha_{sp}$) 1.0 1.0

0 3 3 4.0 1.0

3.0946 0.1237

1.1746 0.4234

0.4578 0.5112

0 3 1 0.0 1.0

0.1781 (α_{d}) 1.0

0 1 1 2.0 1.0

0.1424 ($^{2}\alpha_{sp}$) 1.0 1.0

Oxygen Basis set

8 3

0 0 6 2.0 1.0

5484.671660 0.001831074430

825.2349460 0.01395017220

188.0469580 0.06844507810

52.96450000 0.2327143360

16.89757040 0.4701928980

5.799635340 0.3585208530

0 1 3 6.0 1.0

15.53961625 -0.1107775490 0.07087426820

3.599933586 -0.1480262620 0.3397528390

1.013761750 1.130767010 0.7271585770

0 1 1 0.0 1.0

0.2742 (α_{sp}) 1.0 1.0