

Supplementary Information for “Cost-Effective Hybrid Density Functional Theory Calculation of Three-dimensional Band Structure and Search of Band Edge Positions”

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Table S1. The raw data used to draw Fig. 1. Only the k -point grid and the reduction factor (C) for one direction are denoted, and those for the other two directions are the same. E_{tot} represents the total energy of diamond Si per unit cell (2 atoms).

k -point	C	Max $\Delta\epsilon$	E_{tot}	k -point	C	Max $\Delta\epsilon$	E_{tot}
4	1	0	-12.405	24	4	0.0085	
4	2	0.3231		24	6	0.0487	
4	4	1.0474		24	8	0.1292	
6	1	0	-12.555	24	12	0.3731	
6	2	0.1201		24	24	1.1166	
6	3	0.3638		27	1	0	-12.574
6	6	1.0863		27	3	0.0009	
8	1	0	-12.571	27	9	0.1292	
8	2	0.047		27	27	1.1179	
8	4	0.3712		30	1	0	-12.574
8	8	1.0934		30	2	0.0001	
12	1	0	-12.574	30	3	0.0004	
12	2	0.0084		30	5	0.0093	
12	3	0.0486		30	6	0.0204	
12	4	0.1291		30	10	0.1291	
12	6	0.3731		30	15	0.3731	
12	12	1.1165		30	30	1.1178	
16	1	0	-12.574	32	1	0	-12.574

16	2	0.0017		32	2	0.0001	
16	4	0.0487		32	4	0.0017	
16	8	0.3731		32	8	0.0488	
16	16	1.1174		32	16	0.3731	
18	1	0	-12.574	32	32	1.1174	
18	2	0.0008		34	1	0	-12.574
18	3	0.0091		34	2	0.0001	
18	6	0.1291		34	17	0.3731	
18	9	0.3731		34	34	1.1167	
18	18	1.1161		35	1	0	-12.574
24	1	0	-12.574	35	5	0.0043	
24	2	0.0001		35	7	0.0199	
24	3	0.0019		35	35	1.1164	

Table S2. Mean absolute difference (MAD) and standard deviation (STDEV) of the eigenvalues of diamond Si. Only the k -point grid and the reduction factor (C) for one direction are denoted, while those for the other two directions are the same.

k -point	C	MAD (eV)	STDEV (eV)	k -point	C	MAD (eV)	STDEV (eV)
4	4	0.1514	0.2634	24	6	0.0045	0.0077
4	2	0.0358	0.0647	24	4	0.0007	0.0013
4	1	0	0	24	3	0.0001	0.0003
6	6	0.1519	0.2649	24	2	0.0000	0.0000
6	3	0.0406	0.0704	24	1	0	0
6	2	0.0115	0.0215	27	27	0.1429	0.2515
6	1	0	0	27	9	0.0123	0.0204
8	8	0.1498	0.2614	27	3	0.0001	0.0001
8	4	0.0401	0.0693	27	1	0	0
8	2	0.0042	0.0079	30	30	0.1423	0.2507

8	1	0	0	30	15	0.0370	0.0631
12	12	0.1469	0.2573	30	10	0.0123	0.0202
12	6	0.0392	0.0672	30	6	0.0017	0.0031
12	4	0.0130	0.0220	30	5	0.0007	0.0013
12	3	0.0047	0.0083	30	3	0.0000	0.0001
12	2	0.0006	0.0013	30	2	0.0000	0.0000
12	1	0	0	30	1	0	0
16	16	0.1449	0.2546	32	32	0.1421	0.2503
16	8	0.0383	0.0655	32	16	0.0369	0.0629
16	4	0.0046	0.0080	32	8	0.0044	0.0075
16	2	0.0001	0.0003	32	4	0.0001	0.0003
16	1	0	0	32	2	0.0000	0.0000
18	18	0.1445	0.2539	32	1	0	0
18	9	0.0380	0.065	34	34	0.142	0.2501
18	6	0.0126	0.0211	34	17	0.0368	0.0627
18	3	0.0007	0.0014	34	2	0.0000	0.0000
18	2	0.0001	0.0001	34	1	0	0
18	1	0	0	35	35	0.1744	0.302
24	24	0.1431	0.2519	35	7	0.0304	0.1352
24	12	0.0374	0.0638	35	5	0.01	0.0487
24	8	0.0124	0.0206	35	1	0	0

Table S3. The maximum eigenvalue difference (Max $\Delta\epsilon$) between the full HSE06 calculation and the HSE06 calculation with the reduction factor. The first and the second numbers in the parentheses are the k -point grid and the reduction factor, respectively. For instance, (12,2) indicates that a $12\times 12\times 12$ k -point grid and the reduction factor of 2 were employed. The four highest valence bands and the four lowest conduction bands were used for comparison. The total energy calculated by using a $12\times 12\times 12$ k -point grid was well converged (less than 1 meV per unit cell) for every material. The “PREC” tag was set to “Normal” in the INCAR file. STDEV stands for standard deviation.

Material	Max $\Delta\epsilon(12,2)$	Max $\Delta\epsilon(18,3)$	Max $\Delta\epsilon(24,4)$	Max $\Delta\epsilon(24,2)$	$E_{\text{tot}}(12,1)$	$E_{\text{tot}}(18,1)$	$E_{\text{tot}}(24,1)$
AlAs	0.0048	0.0050	0.0048	0.0001	-10.986	-10.986	-10.986
AlP	0.0035	0.0035	0.0035	0.0001	-12.026	-12.026	-12.026

AlSb	0.0055	0.0062	0.0056	0.0001	-9.823	-9.824	-9.824
BAs	0.0076	0.0085	0.0076	0.0001	-13.282	-13.282	-13.282
BP	0.0068	0.0078	0.0068	0.0001	-14.865	-14.865	-14.865
C	0.0064	0.0061	0.0064	0.0001	-21.105	-21.105	-21.106
CdO	0.0065	0.0065	0.0065	0.0001	-10.042	-10.042	-10.042
GaAs	0.0116	0.0120	0.0120	0.0004	-9.933	-9.933	-9.933
CdTe	0.0040	0.0041	0.0041	0.0001	-6.031	-6.031	-6.031
GaP	0.0065	0.0073	0.0065	0.0001	-10.833	-10.833	-10.833
GaSb	0.0135	0.0142	0.0143	0.0007	-8.985	-8.985	-8.985
Ge	0.0182	0.0193	0.0207	0.0012	-10.696	-10.696	-10.696
HgSe	0.0090	0.0138	0.0157	0.0013	-5.269	-5.269	-5.269
HgTe	0.0086	0.0133	0.0147	0.0010	-4.714	-4.715	-4.715
InAs	0.0121	0.0128	0.0129	0.0008	-9.234	-9.234	-9.234
InP	0.0072	0.0074	0.0074	0.0002	-9.961	-9.961	-9.961
InSb	0.0115	0.0122	0.0125	0.0007	-8.471	-8.471	-8.471
Sn	0.0155	0.0206	0.0215	0.0016	-9.056	-9.057	-9.057
ZnS	0.0021	0.0021	0.0021	0.0001	-8.379	-8.379	-8.379
ZnSe	0.0038	0.0038	0.0038	0.0001	-7.436	-7.436	-7.436
ZnTe	0.0044	0.0045	0.0045	0.0001	-6.444	-6.444	-6.444
Average	0.0081	0.0091	0.0092	0.0004			
STDEV	0.0043	0.0052	0.0057	0.0005			

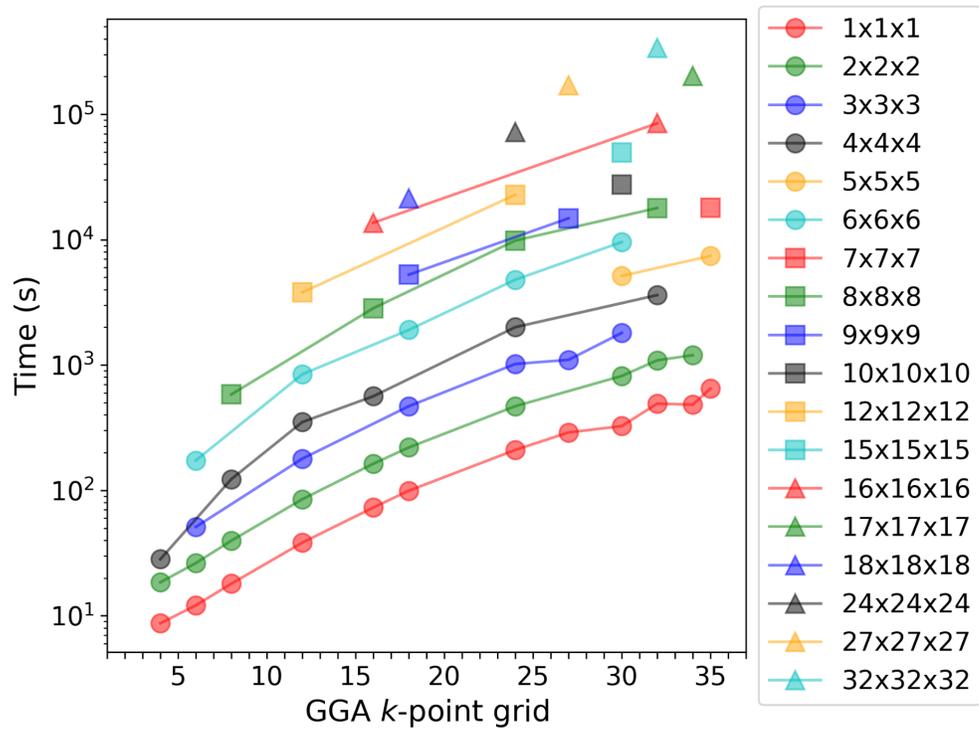


Figure S1. Calculation time to obtain data in Figure 1. Data points are distinguished according to the Hartree-Fock (HF) k -point grid. For a given GGA k -point grid, we performed self-consistent field (SCF) calculations using a smaller HF grid and increased the HF grid. It means that most of the data were obtained by several steps.

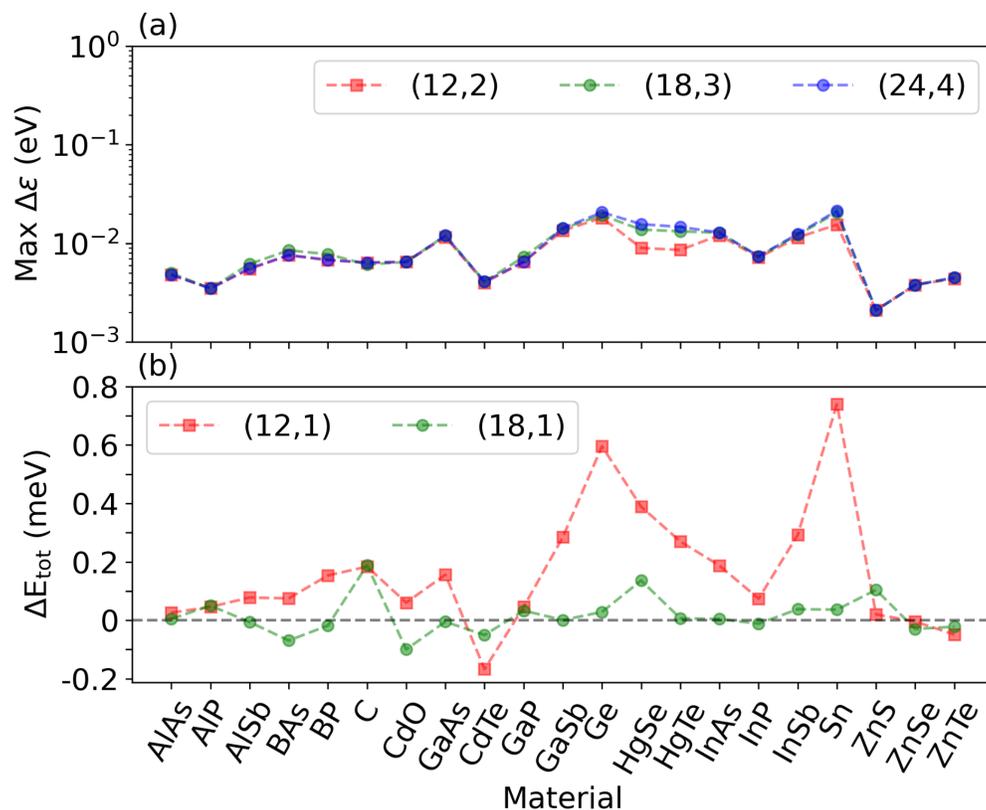


Figure S2. The maximum eigenvalue difference ($\text{Max } \Delta\epsilon$) between the full HSE06 calculation and the HSE06 calculation with the reduction factor. Data identical to those in Table S3. (a) $\text{Max } \Delta\epsilon$ does not change much as the k -point grid for the Fock exchange potential is equivalent. (b) ΔE_{tot} is the total energy with respect to $\Delta E_{\text{tot}}(24,1)$.