Supplementary material of "Assessing the performance of exchange-correlation functionals on lattice constants of binary solids at room temperature within quasi-harmonic approximation"

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No.	Comp.	Space group	LDA	PBE	PBEsol	r2SCAN	SCAN	rSCAN	E _g exp.
1	MgO	$Fm\bar{3}m$	0	0	0	0	0	0	7.9
2	MgS	$Fm\bar{3}m$	0	0	0	0	0	0	4.5
3	MgSe	$Fm\bar{3}m$	0	0	0	0	0	0	4.05
4	CaO	$Fm\bar{3}m$	0	0	0	0	4	0	7.8
5	CaS	$Fm\bar{3}m$	0	0	0	0	1	0	3.9
6	CaSe	$Fm\bar{3}m$	0	0	0	0	3	0	3.81
7	CdO	$Fm\bar{3}m$	0	0	0	0	0	0	0.84
8	SrO	$Fm\bar{3}m$	Ő	Ő	Õ	Ő	Ő	Ő	5.22
9	SrS	$Fm\bar{3}m$	Ő	Ő	Õ	Ő	Ő	Ő	4 10
10	SrSe	$Fm\bar{3}m$	Ő	Ő	Ő	0 0	0	0	3 71
11	SrTe	$Fm\bar{3}m$	Ő	Ő	Ő	Õ	0	Ő	2.57
12	BaSe	$Fm\bar{3}m$	0	0	0	0	0	0	3.58
13	TiC	$Fm\bar{3}m$	0	0	0	0	0	0	0.00
14		$Fm\bar{3}m$	0	0	0	0	0	0	0.00
14	HfC	$Fm\bar{3}m$	0	0	0	0	0	0	0.00
16	$7_{n}\mathbf{N}$	$Fm\bar{3}m$	0	0	0	0	0	0	0.00
10	LIIN	$F m \overline{2} m$	0	0	0	0	0	0	0.00
10	HIN Car A a	F m3m E2	0	1	0	1	0	0	0.00
18	ShAs	Fm3m	0	1	0	1	4	2	0.00
19	SCN	Fm3m	0	0	0	0	0	0	1.3
20	SCP	Fm3m	0	0	0	0	2	0	0.00
21	ScAs	Fm3m	0	0	0	0	0	0	0.00
22	ScSb	Fm3m	0	0	0	0	3	1	0.00
23	ScB1	Fm3m	0	0	0	0	4	0	0.00
24	ΥN	Fm3m	0	0	0	0	0	0	0.5
25	ΥP	$Fm\underline{3}m$	0	0	0	0	0	0	1.0
26	YAs	$Fm\underline{3}m$	0	0	0	0	0	0	0.0
27	YSb	$Fm\underline{3}m$	0	0	0	0	0	0	0.0
28	YBi	$Fm\underline{3}m$	0	0	0	0	0	0	0.0
29	LaP	$Fm\overline{3}m$	0	0	0	0	0	0	0.56
30	NaCl	$Fm\overline{3}m$	0	0	0	5	4	5	8.50
31	BeS	$F\overline{4}3m$	0	0	0	0	0	0	5.50
32	BeSe	$F\bar{4}3m$	0	0	0	0	0	0	5.60
33	BeTe	$F\bar{4}3m$	0	0	0	0	0	0	2.80
34	ZnS	$F\bar{4}3m$	0	0	0	3	5	0	3.72
35	ZnSe	$F\bar{4}3m$	0	0	0	7	5	5	2.82
36	ZnTe	$F\bar{4}3m$	0	0	0	7	5	5	2.35
37	CdSe	$F\bar{4}3m$	1	0	1	2	6	0	1.90
38	CdTe	$F\bar{4}3m$	1	0	0	0	3	0	1.92
39	BN	$F\bar{4}3m$	0	0	0	0	0	0	6.22
40	BP	$F\bar{4}3m$	0	0	0	0	0	0	2.40
41	BAs	$F\bar{4}3m$	0	0	0	0	0	0	1.46
42	AlP	$F\bar{4}3m$	0	0	0	0	0	0	2.51
43	AlAs	$F\bar{4}3m$	0	0	0	0	0	0	2.23
44	AlSb	$F\bar{4}3m$	0	0	0	0	0	0	1.68
45	GaN	$F\bar{4}3m$	0	0	0	0	1	5	3.30
46	GaP	$F\bar{4}3m$	0	0	0	2	6	0	2.35
47	GaAs	$F\bar{4}3m$	0	0	0	0	1	3	1.52
48	GaSb	$F\bar{4}3m$	0	0	1	7	2	1	0.73
49	InP	$F\bar{4}3m$	0	0	0	0	3	1	1.42
50	InAs	$F\bar{4}3m$	0	0	0	0	3	1	0.41
51	InSb	$F\bar{4}3m$	0	0	1	0	2	0	0.23
52	SiC	$F\bar{4}3m$	0	0	0	0	0	0	2.42
53	CaF ₂	$Fm\bar{3}m$	0	0	0	0	5	0	12.6
54	SrF_{2}	$Fm\bar{3}m$	Ő	Ő	Ō	Ő	4	ů 0	11.2
55	BaF_2	$Fm\bar{3}m$	0	0	0	3	3	0	10.6

Table 1: The number of imaginary frequencies of each compound with different functionals.

56	CdF_2	$Fm\bar{3}m$	0	3	1	2	3	1	7.6
57	ScCu	$Pm\bar{3}m$	3	0	0	3	6	6	0.00
58	YCu	$Pm\bar{3}m$	2	0	0	2	8	6	0.00
59	YAg	$Pm\bar{3}m$	3	0	0	0	2	0	0.00
60	MgSc	$Pm\bar{3}m$	0	0	0	0	6	5	0.00

Table 2: The \mathbb{R}^2 value of fitting Murnaghan equation of state using DFT energy (E) and Helmholtz free energy (HFE). The symbol '/' indicates the failure of EOS fitting.

No. Comp. E IFFE IFFE <th></th> <th colspan="2">LDA</th> <th colspan="2">PBE</th> <th colspan="2">PBEsol</th> <th colspan="2">r²SCAN</th> <th colspan="2">SCAN</th> <th colspan="2">rSCAN</th>		LDA		PBE		PBEsol		r ² SCAN		SCAN		rSCAN		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	No.	Comp.	E	HFE	E	HFE	E	HFE	E	HFE	E	HFE	E	HFE
1 MgO 1.00000 1.00000 1.00000 1.00000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 </td <td></td>														
2 MgS 1.00000 1.00000 1.00000 1.00000 0.00000<	1	MgO	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99987	1.00000	0.99997	1.00000	1.00000
3 Agesc 1.00000 1.0000	2	MgS	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99940	1.00000	0.99946	1.00000	1.00000
a c.s.s. 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 0.000	3	MgSe	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99906	1.00000	0.99946	1.00000	1.00000
6 Corss. 1.00000 1.00000 1.00000 1.00000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 0.0000 0.99998 1.00000 0.99894 1.00000 0.99894 1.00000 0.99894 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99996 1.00000 0.99999 1.00000 0.99999 1.00000 <td< td=""><td>4</td><td>CaO</td><td>1.00000</td><td>1.00000</td><td>1.00000</td><td>1.00000</td><td>1.00000</td><td>1.00000</td><td>1.00000</td><td>1.00000</td><td>0.99971</td><td>0.98097</td><td>0.99994</td><td>0.99887</td></td<>	4	CaO	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99971	0.98097	0.99994	0.99887
7 CAC0 1.00000 0.09999 1.00000 0.09999 1.00000 0.09998 1.00000 0.09998 1.00000 0.09908 1.00000 0.09908 1.00000 0.09908 1.00000 0.09908 1.00000 0.09908 1.00000 0.09908 1.00000 0.99908 1.00000	6	CaSe	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99995	0.00090	0.999999	0.99110
s SrO Longen 0.99999 Longen Longen <thlongen< <thlongen<="" th="" thcm=""> <thlongen< th=""></thlongen<></thlongen<>	7	CdO	1.00000	0.99995	1.00000	0.99998	1.00000	0.99998	1.00000	0.99990	1.00000	0.99886	1.00000	1.00000
9 S:S: 1 00000 1 00000 1 00000 1 00000 0 09968 1 00000 0 00000 1 00000 1 00000 1 00000 1 00000 0 00000 1 00000	8	SrO	1.00000	0.99999	1.00000	0.99997	1.00000	0.99999	1.00000	1.00000	1.00000	0.99996	1.00000	1.00000
10 SrSe 1.00000 1.00000 1.00000 1.00000 0.00000 0.00000 0.00000 1.00000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	9	SrS	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99994	1.00000	0.99068	1.00000	1.00000
11 SrTe 1.00000 1.00000 1.00000 1.00000 0.00000 1.0000	10	SrSe	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99978	1.00000	0.99874	1.00000	1.00000
12 BaSe 1.00000 0.00000 1.00000 1.00000 0.0000 0.0000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000 <td>11</td> <td>SrTe</td> <td>1.00000</td> <td>1.00000</td> <td>1.00000</td> <td>1.00000</td> <td>1.00000</td> <td>1.00000</td> <td>1.00000</td> <td>0.99957</td> <td>1.00000</td> <td>0.99967</td> <td>1.00000</td> <td>1.00000</td>	11	SrTe	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99957	1.00000	0.99967	1.00000	1.00000
13 TC 1.00000 0.00000 1.00000 0.00000<	12	BaSe	1.00000	0.99999	1.00000	1.00000	1.00000	1.00000	1.00000	0.99991	1.00000	0.99906	1.00000	1.00000
14 ZrC 1.00000	13	TiC	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99997	0.99711	0.99975	0.99948
Inc 1.00000 1.	14	ZrC	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99984
10 21X 1,00000	15	HfC Z-N	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	10	LIIN	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.999999
13 Sinks 1.00000 0.00000 1.00000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000	18	SnAc	1.00000	1.00000	1.00000	0.00007	1.00000	0.00004	1.00000	0.999999	0.00000	0.06470	0.00000	0.999990
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	10	ScN	1.00000	1 00000	1.00000	1 00000	1.00000	1 00000	1.00000	0.99985	1 00000	0.90479	0.999999	0.98925
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	20	ScP	1.00000	1.00000	1.00000	1.00000	1.00000	0.99995	1.00000	0.999999	1.00000	0.97731	0.999999	0.99495
22 ScSb 1.00000 0.99999 1.00000 1.00000 0.99871 0.99990 0.97045 0.99997 0.97437 24 YN 1.00000 0.99981 1.00000 1.00000 1.00000 1.00000 0.99981 0.00000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.0000 0.99991 0.99911 0.0000 0.99911 0.0000 0.99911 0.0000 0.99911 0.0000 0.99911 0.0000 0.99911 0.0000 0.99911 0.0000 0.99911 0.0000 0.99911 0.0000 0.99911 0.0000 0.99911 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.000	21	ScAs	1.00000	0.99996	1.00000	0.99999	1.00000	1.00000	1.00000	0.99968	0.99998	0.96093	0.999999	0.99138
32 ScBi 1.00000 0.99984 1.00000 0.99987 0.99987 0.97045 0.99997 0.97437 24 YN 1.00000 0.99984 1.00000 1.00000 1.00000 1.00000 0.99984 1.00000 0.00000 25 YP 1.00000 0.0000 1.00000 1.00000 1.00000 1.00000 0.0000	22	ScSb	1.00000	0.99999	1.00000	1.00000	1.00000	1.00000	1.00000	0.99990	1.00000	0.98602	0.99998	0.99444
24 YN 1.00000 0.99984 1.00000 0.99994 1.00000 0.00000 25 YP 1.00000 0.00000 1.00000 1.00000 1.00000 1.00000 0.99984 1.00000 0.99934 1.00000 1.00000 26 YAs 1.00000 0.99995 1.00000 1.00000 1.00000 1.00000 1.00000 0.99984 1.00000 0.99984 1.00000 0.99996 0.9313 1.00000 1.00000 1.00000 1.00000 0.99997 0.99158 0.7317 0.99986 0.7317 0.99986 0.7317 0.99996 0.97317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996 0.7317 0.99996<	23	ScBi	1.00000	0.99999	1.00000	0.99997	1.00000	0.99994	1.00000	0.99887	0.99999	0.97045	0.99997	0.97437
25YP1.000001.000001.000001.000001.000001.000001.000000.00000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.00000.00000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.000000.00000 <td>24</td> <td>YN</td> <td>1.00000</td> <td>0.99984</td> <td>1.00000</td> <td>1.00000</td> <td>1.00000</td> <td>1.00000</td> <td>1.00000</td> <td>0.99998</td> <td>1.00000</td> <td>0.99994</td> <td>1.00000</td> <td>1.00000</td>	24	YN	1.00000	0.99984	1.00000	1.00000	1.00000	1.00000	1.00000	0.99998	1.00000	0.99994	1.00000	1.00000
26 YAs 1.00000 0.09000 1.00000 1.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.99981 1.00000 0.99881 1.00000 0.99881 1.00000 0.99881 1.00000 0.99881 1.00000 0.99881 1.00000 0.99980 0.7024 30 RaC1 1.00000 0.99974 1.00000 <	25	YP	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99845	1.00000	1.00000
27YSb1.000001.000001.000001.000001.000001.000000.999911.000000.999911.000000.999911.000000.999911.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999151.000000.999150.999970.992880.792410.999460.9702430BeS1.000001.000001.000001.000001.000001.000001.000001.000000.999491.000000.999491.000000.999361.000000.999361.000000.999360.999990.98660.99997/1.000000.937341.000000.998520.999990.986640.99997/1.000000.937341.000000.987411.000000.987411.000000.998581.000000.998531.000000.999531.000000.999531.000000.999531.000000.999531.000000.999531.000000.999531.000000.999531.000000.999531.000000.999531.000000.999531.000000.999531.000000.999531.000000.999531.000000.995531.000000.999531.000000.995531.000000.999531.000000.995531.000000.995531.000000.995531.000000.995531.000001.0	26	YAs	1.00000	0.99995	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99382	1.00000	1.00000
28 YBi 1.00000 0.99999 1.00000 0.99993 1.00000 0.99913 1.00000 0.99915 0.00000 0.99915 0.00000 0.99915 0.00000 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99915 0.99910 0.99126 0.99100	27	YSb	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99999	0.99891	1.00000	1.00000
129 LaP 1.00000 1.00000 1.00000 1.00000 1.00000 0.09958 0.30000 0.39998 0.30000 0.39998 0.30000 0.39998 0.30000 0.39998 0.30000 0.39999 0.3668 0.39977 1.00000 0.39358 1.00000 0.39358 1.00000 0.39356 1.30000 0.39939 0.3666 0.39939 0.38451 1.00000 0.39356 1.30000 0.39358 1.00000 0.39358 1.00000 0.39356 1.30000 0.39358 1.00000 0.39358 1.00000 0.39358 1.00000 0.30001<	28	YBi	1.00000	0.99999	1.00000	0.99996	1.00000	0.99997	1.00000	0.99993	1.00000	0.99313	1.00000	1.00000
30 NAC1 1.00000 0.99944 1.00000 0.99958 0.19928 0.19928 0.19928 0.19928 0.19928 0.19928 0.19928 0.19928 0.19928 0.19928 0.10000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 0.99983 1.00000 0.99993 1.00000 1.0000	29	LaP	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99580	1.00000	0.99988
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	30 20	NaCI DoS	1.00000	0.99974	1.00000	0.99890	1.00000	0.99915	0.99997	0.99288	0.99958	0.73917	0.99996	1.00000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	30 39	BeSe	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99540	1.00000	1.00000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	33	BeTe	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.999999	1.00000	1.00000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	34	ZnS	1.00000	0.99995	1.00000	0.99997	1.00000	0.99982	0.999999	0.99686	0.99997	/	1.00000	0.93396
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	35	ZnSe	1.00000	0.99970	1.00000	0.99907	1.00000	0.99952	0.999999	0.94604	0.99990	0.99388	1.00000	0.98740
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	36	ZnTe	1.00000	0.99879	1.00000	0.99788	1.00000	0.99906	0.99999	0.89794	1.00000	0.95696	1.00000	0.99985
38CdTe1.000000.999611.000000.999261.000000.999121.000000.999901.000000.963921.000000.9999839BN1.000001.000001.000001.000001.000001.000001.000001.000000.999991.000000.999991.000000.999991.000000.999991.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999091.000000.999141.000001.000001.000000.999141.000001.000001.000000.999181.000000.999121.000000.999121.000000.999121.000000.999121.000000.999121.000000.999141.000001.000001.000001.000001.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999131.000000.999141.000000.999141.0000	37	CdSe	1.00000	0.99971	1.00000	0.99936	1.00000	0.99961	1.00000	0.99922	1.00000	0.89495	1.00000	0.99996
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	38	CdTe	1.00000	0.99961	1.00000	0.99926	1.00000	0.99912	1.00000	0.99990	1.00000	0.96392	1.00000	0.99998
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	39	BN	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99999	1.00000	1.00000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	40	BP	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99671	1.00000	1.00000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	41	BAs	1.00000	0.99999	1.00000	0.99999	1.00000	0.99999	1.00000	1.00000	1.00000	0.99902	1.00000	1.00000
43AIAs1.000001.000001.000001.000001.000001.000001.000000.999921.000000.999941.000001.0000044AlSb1.000001.000001.000001.000001.000001.000001.000000.999921.000000.999921.000000.999921.000000.999921.000000.999931.000000.999931.000000.999961.000000.999970.982920.999900.9923347GaAs1.000000.999831.000000.999931.000000.999950.999970.98880.987231.00000.999990.9923347GaAs1.000000.999801.000000.999431.000000.999431.000000.999930.999720.998880.987231.00000.999990.9923349InP1.000000.999931.000000.999721.000000.999771.000000.998631.000000.998631.000000.9981250InAs1.000000.999731.000000.999721.000000.999821.000000.998831.000000.998831.000000.998831.000000.998831.000000.998641.000000.998641.000000.998641.000000.998641.000000.998641.000000.998631.000000.998631.000000.998631.000000.998631.000000.998631.000000.998631.000000.998631.000000.998631.00	42	AIP	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99823	1.00000	0.99657	1.00000	1.00000
44ARSD1.000001.000001.000001.000001.000001.000001.000000.999981.000000.999921.000000.999920.999920.999920.999920.999920.9991646GaP1.000000.999961.000000.999931.000000.999961.000000.999960.999990.98220.999990.999220.999990.9923347GaAs1.000000.999831.000000.999481.000000.999960.999970.999720.98880.987231.00000/48GaSb1.000000.999831.000000.999631.000000.999971.000000.995291.000000.995670.999990.9639149InP1.000000.999931.000000.999771.000000.999771.000000.99861.000000.988301.000000.9981250InAs1.000000.999701.000000.999721.000000.999751.000000.998311.000000.9984151InSb1.000001.000001.000001.000001.000001.000001.000001.000001.000001.000000.9999553CaF21.000000.999871.000000.999951.000000.999951.000000.999961.000000.999651.0000055BaF21.000000.999841.000000.999841.000000.999861.000000.999990.9525758MgSc	43	AIAS	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99982	1.00000	0.99994	1.00000	1.00000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	44	GaN	1.00000	0.00000	1.00000	0.00000	1.00000	0.00000	1.00000	0.99908	0.00000	0.99932	0.00000	0.00160
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	46	GaP	1.00000	0.333333	1.00000	0.333333	1.00000	0.999999	1.00000	0.333300	0.999999	0.98299	0.99902	0.33100
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	47	GaAs	1.00000	0.99883	1.00000	0.99948	1.00000	0.99965	0.999999	0.99972	0.99888	0.98723	1.00000	/
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	48	GaSb	1.00000	0.99980	1.00000	0.99963	1.00000	0.99992	1.00000	0.99529	1.00000	0.99567	0.999999	0.96391
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	49	InP	1.00000	0.99993	1.00000	0.99997	1.00000	0.99997	1.00000	0.99986	1.00000	0.98030	1.00000	0.99812
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	50	InAs	1.00000	0.99975	1.00000	0.99972	1.00000	0.99975	1.00000	0.99893	1.00000	0.98581	1.00000	0.99143
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	51	InSb	1.00000	0.99970	1.00000	0.99952	1.00000	0.99982	1.00000	0.99980	1.00000	0.97448	1.00000	0.93647
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	52	SiC	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	0.99988	1.00000	1.00000
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	53	CaF_2	1.00000	0.99993	1.00000	0.99995	1.00000	0.99995	1.00000	0.99975	0.99999	0.95355	0.99999	0.99422
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	54	SrF_2	1.00000	0.99987	1.00000	0.99984	1.00000	0.99992	1.00000	0.99996	1.00000	0.99965	1.00000	1.00000
56 CdF2 1.00000 0.99967 1.00000 0.99995 1.00000 0.99980 1.00000 0.99992 0.99996 0.98148 1.00000 0.99999 57 ScCu 1.00000 0.99831 1.00000 0.99978 1.00000 0.99974 1.00000 0.98255 0.99993 0.92073 0.99999 0.95557 58 MgSc 1.00000 0.99994 1.00000 0.99994 1.00000 0.99996 0.90995 0.99995 0.99662 0.99889 0.94249 59 YCu 1.00000 0.99920 1.00000 0.99931 1.00000 0.99995 0.99970 0.74416 1.0 / 60 YAg 1.00000 0.99984 1.00000 0.99992 1.00000 0.99999 0.99999 0.99999 0.99999 0.99999 0.99999 0.99970 0.74416 1.0 /	55	BaF_2	1.00000	0.99894	1.00000	0.99686	1.00000	0.99841	1.00000	0.99967	1.00000	0.99824	1.00000	1.00000
57 ScCu 1.00000 0.99831 1.00000 0.99978 1.00000 0.99974 1.00000 0.98925 0.99993 0.92073 0.99999 0.95557 58 MgSc 1.00000 0.99994 1.00000 0.99994 1.00000 0.99996 1.00000 0.999995 0.99995 0.99962 0.99989 0.92073 0.99989 0.92073 0.999999 0.99999 0.999993 0.99999 0.999993 0.99962 0.99989 0.99989 0.99999 0.99995 0.999993 0.99966 0.999993 0.99966 0.999993 0.99966 0.999993 0.99966 0.99994 1.00000 0.99994 1.00000 0.999959 0.999993 0.99970 0.74416 1.0 / 60 YAg 1.00000 0.99994 1.00000 0.99994 1.00000 0.999996 0.999996 0.999999 0.999999 0.999999 0.999999 0.999997	56	CdF_2	1.00000	0.99967	1.00000	0.99995	1.00000	0.99980	1.00000	0.99992	0.99996	0.98148	1.00000	0.999999
58 Mg3c 1.00000 0.99994 1.00000 0.99994 0.99995 0.99995 0.99995 0.99995 0.99995 0.99995 0.99995 0.99997 0.74416 1.0 / 60 YAg 1.00000 0.99986 1.00000 0.99994 1.00000 0.99992 1.00000 0.99997 0.74416 1.0 /	57 E0	ScCu Mrs	1.00000	0.99831	1.00000	0.99978	1.00000	0.99974	1.00000	0.98925	0.99993	0.92073	0.99999	0.95557
60 YAg 1.00000 0.99986 1.00000 0.99994 1.00000 0.99992 1.00000 0.99996 0.99999 0.98580 1.00000 0.99997	98 50	Mg5c VCu	1.00000	0.99994	1.00000	0.99994	1.00000	0.99990	1.00000	0.999999	0.99999 0.00070	0.99002	0.99989	0.94249
The second courses and	60	YAg	1.00000	0.99986	1.00000	0.99994	1.00000	0.99992	1.00000	0.99996	0.99999	0.98580	1.00000	0.99997

Comp	IDA	DDE	DDEcol	SCAN	"SCAN	2SCAN	0110
Comp.		PDE	PDESO	SUAN	ISCAN	r-SCAN	exp
MgO	1.57	1.67	1.62	1.65	1.63	1.41	1.53
CaO	1.60	1.72	1.67	/	1.23	1.59	1.57
SrO	1.64	1.81	1.74	1.91	1.64	1.63	1.52
TiC	1.55	1.64	1.57	1.51	2.00	1.67	1.72
ZrC	1.57	1.65	1.59	1.76	1.66	1.67	1.35
HfC	1.58	1.67	1.60	1.97	1.67	1.70	1.61
SiC	0.71	0.75	0.72	0.43	0.75	0.74	0.75
BN	0.84	0.88	0.85	0.83	0.90	0.89	0.70
BP	0.70	0.73	0.69	0.44	0.75	0.73	0.75
BAs	0.81	0.82	0.80	0.51	0.85	0.84	0.75
AlP	0.46	0.55	0.46	0.38	0.57	0.32	0.75
AlAs	0.55	0.63	0.54	0.64	0.65	0.44	0.66
AlSb	0.51	0.61	0.50	0.27	0.63	0.78	0.60
InP	0.64	0.80	0.75	1.41	0.84	0.75	0.60
InAs	0.46	0.87	0.48	0.65	/	0.93	0.57
InSb	0.57	0.71	0.81	1.39	2.49	0.87	0.56
BaF_2	1.59	2.54	1.25	2.33	1.71	1.74	1.59
SrF_2	1.80	1.79	1.92	1.36	1.73	1.83	1.59
CaF_2	1.86	1.87	1.91	1.27	1.93	1.66	1.73

Table 3: DFT Calculated Grüneisen parameters at 300 K with different functionals, comparing with experiment values.

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Figure S1: Comparison of the zero-point correction (the difference between the ZPE-corrected lattice constants and non-ZPE-corrected ones) between the previous work (Zhang *et al.* Ref. [4]) and our work (this work) with four different functionals.



Figure S2: The difference (Δa) between the ZPE-corrected lattice constants and non-ZPE-corrected ones with six functionals used in this work.



Figure S3: The relative error of lattice constants calculated using different functionals with ZPE correction with respect to experimental values.



Figure S4: The relative error of DFT calculated lattice constants at 300 K with respect to experimental values at room temperature.



Figure S5: Relative errors of lattice constants computed at 0K with respect to experiment values at room temperature.



Figure S6: Correlation between the relative errors of DFT calculated lattice constants at 300 K within the QHA with respect to the experimental values at room temperature and formation energy adapted from the OQMD [5], bulk modulus, Grüneisen parameter at room temperature, and band gaps calculated by PBEsol.



Figure S7: The compounds with poor equation of state fitting $(R^2 \leq 0.995)$ for Helmholtz free energy using SCAN.



Figure S8: The compounds with poor equation of state fitting $(R^2 \leq 0.995)$ for Helmholtz free energy using rSCAN and r²SCAN.



Figure S9: Phonon spectra of YCu calculated by LDA, PBE, PBEsol, SCAN, rSCAN, and r²SCAN. The negative frequency indicates an imaginary frequency.



Figure S10: Phonon spectra of PbTe calculated at 0 K and 0.1 K using SCAN functional.