# 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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June 23, 2023

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

| 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 | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 5.22 |
| 9 | SrS | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 4.10 |
| 10 | SrSe | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 3.71 |
| 11 | SrTe | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 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 | ZrC | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.00 |
| 15 | HfC | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.00 |
| 16 | ZrN | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.00 |
| 17 | HfN | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.00 |
| 18 | SnAs | $Fm\bar{3}m$ | 0 | 1 | 0 | 1 | 4 | 2 | 0.00 |
| 19 | ScN | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 1.3 |
| 20 | ScP | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 2 | 0 | 0.00 |
| 21 | ScAs | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.00 |
| 22 | ScSb | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 3 | 1 | 0.00 |
| 23 | ScBi | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 4 | 0 | 0.00 |
| 24 | YN | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.5 |
| 25 | YP | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 1.0 |
| 26 | YAs | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.0 |
| 27 | YSb | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.0 |
| 28 | YBi | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.0 |
| 29 | LaP | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.56 |
| 30 | NaCl | $Fm\bar{3}m$ | 0 | 0 | 0 | 5 | 4 | 5 | 8.50 |
| 31 | BeS | $F\bar{4}3m$ | 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 | $SrF_2$ | $Fm\bar{3}m$ | 0 | 0 | 0 | 0 | 4 | 0 | 11.2 |
| 55 | $BaF_2$ | $Fm\bar{3}m$ | 0 | 0 | 0 | 3 | 3 | 0 | 10.6 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 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 $R^2$ value of fitting Murnaghan equation of state using DFT energy ($E$) and Helmholtz free energy (HFE). The symbol '/' indicates the failure of EOS fitting.

| | | LDA | | PBE | | PBEsol | | r$^2$SCAN | | SCAN | | rSCAN | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| No. | Comp. | $E$ | HFE | $E$ | HFE | $E$ | HFE | $E$ | HFE | $E$ | HFE | $E$ | HFE |
| 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 |
| 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 |
| 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 |
| 4 | CaO | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99971 | 0.98697 | 0.99994 | 0.99887 |
| 5 | CaS | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99995 | 0.86090 | 0.99999 | 0.99110 |
| 6 | CaSe | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99998 | 0.92938 | 0.99999 | 0.97485 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 15 | HfC | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 |
| 16 | ZrN | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99999 |
| 17 | HfN | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99999 | 1.00000 | 1.00000 | 1.00000 | 0.99996 |
| 18 | SnAs | 1.00000 | 0.99983 | 1.00000 | 0.99997 | 1.00000 | 0.99994 | 1.00000 | 0.99983 | 0.99999 | 0.96479 | 0.99999 | 0.98923 |
| 19 | ScN | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99997 | 1.00000 | 0.99599 | 0.99999 | 0.99930 |
| 20 | ScP | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99995 | 1.00000 | 0.99999 | 1.00000 | 0.97731 | 0.99999 | 0.99495 |
| 21 | ScAs | 1.00000 | 0.99996 | 1.00000 | 0.99999 | 1.00000 | 1.00000 | 1.00000 | 0.99968 | 0.99998 | 0.96093 | 0.99999 | 0.99138 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 30 | NaCl | 1.00000 | 0.99974 | 1.00000 | 0.99890 | 1.00000 | 0.99915 | 0.99997 | 0.99288 | 0.99958 | 0.73917 | 0.99996 | 0.97024 |
| 30 | BeS | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99346 | 1.00000 | 1.00000 |
| 32 | BeSe | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99999 | 1.00000 | 1.00000 |
| 33 | BeTe | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99883 | 1.00000 | 1.00000 |
| 34 | ZnS | 1.00000 | 0.99995 | 1.00000 | 0.99997 | 1.00000 | 0.99982 | 0.99999 | 0.99686 | 0.99997 | / | 1.00000 | 0.93396 |
| 35 | ZnSe | 1.00000 | 0.99970 | 1.00000 | 0.99907 | 1.00000 | 0.99952 | 0.99999 | 0.94604 | 0.99990 | 0.99388 | 1.00000 | 0.98740 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 42 | AlP | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99823 | 1.00000 | 0.99657 | 1.00000 | 1.00000 |
| 43 | AlAs | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99982 | 1.00000 | 0.99994 | 1.00000 | 1.00000 |
| 44 | AlSb | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 1.00000 | 0.99968 | 1.00000 | 0.99952 | 1.00000 | 1.00000 |
| 45 | GaN | 1.00000 | 0.99999 | 1.00000 | 0.99999 | 1.00000 | 0.99999 | 1.00000 | 0.99956 | 0.99999 | 0.98299 | 0.99982 | 0.99160 |
| 46 | GaP | 1.00000 | 0.99996 | 1.00000 | 0.99993 | 1.00000 | 0.99996 | 1.00000 | 0.97908 | 0.99997 | 0.98922 | 0.99999 | 0.99233 |
| 47 | GaAs | 1.00000 | 0.99883 | 1.00000 | 0.99948 | 1.00000 | 0.99965 | 0.99999 | 0.99972 | 0.99888 | 0.98723 | 1.00000 | / |
| 48 | GaSb | 1.00000 | 0.99980 | 1.00000 | 0.99963 | 1.00000 | 0.99992 | 1.00000 | 0.99529 | 1.00000 | 0.99567 | 0.99999 | 0.96391 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 | 0.99999 |
| 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 | 0.99999 | 0.99995 | 0.99662 | 0.99989 | 0.94249 |
| 59 | YCu | 1.00000 | 0.99920 | 1.00000 | 0.99831 | 1.00000 | 0.99959 | 0.99999 | 0.99706 | 0.99970 | 0.74416 | 1.0 | / |
| 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 |

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

| Comp. | LDA | PBE | PBEsol | SCAN | rSCAN | r$^2$SCAN | exp. |
|---|---|---|---|---|---|---|---|
| MgO | 1.57 | 1.67 | 1.62 | 1.65 | 1.63 | 1.41 | 1.53[1] |
| CaO | 1.60 | 1.72 | 1.67 | / | 1.23 | 1.59 | 1.57[1] |
| SrO | 1.64 | 1.81 | 1.74 | 1.91 | 1.64 | 1.63 | 1.52[1] |
| TiC | 1.55 | 1.64 | 1.57 | 1.51 | 2.00 | 1.67 | 1.72[2] |
| ZrC | 1.57 | 1.65 | 1.59 | 1.76 | 1.66 | 1.67 | 1.35[2] |
| HfC | 1.58 | 1.67 | 1.60 | 1.97 | 1.67 | 1.70 | 1.61[2] |
| SiC | 0.71 | 0.75 | 0.72 | 0.43 | 0.75 | 0.74 | 0.75[1] |
| BN | 0.84 | 0.88 | 0.85 | 0.83 | 0.90 | 0.89 | 0.70[1] |
| BP | 0.70 | 0.73 | 0.69 | 0.44 | 0.75 | 0.73 | 0.75[1] |
| BAs | 0.81 | 0.82 | 0.80 | 0.51 | 0.85 | 0.84 | 0.75[1] |
| AlP | 0.46 | 0.55 | 0.46 | 0.38 | 0.57 | 0.32 | 0.75[1] |
| AlAs | 0.55 | 0.63 | 0.54 | 0.64 | 0.65 | 0.44 | 0.66[1] |
| AlSb | 0.51 | 0.61 | 0.50 | 0.27 | 0.63 | 0.78 | 0.60[1] |
| InP | 0.64 | 0.80 | 0.75 | 1.41 | 0.84 | 0.75 | 0.60[1] |
| InAs | 0.46 | 0.87 | 0.48 | 0.65 | / | 0.93 | 0.57[1] |
| InSb | 0.57 | 0.71 | 0.81 | 1.39 | 2.49 | 0.87 | 0.56[1] |
| $BaF_2$ | 1.59 | 2.54 | 1.25 | 2.33 | 1.71 | 1.74 | 1.59[3] |
| $SrF_2$ | 1.80 | 1.79 | 1.92 | 1.36 | 1.73 | 1.83 | 1.59[3] |
| $CaF_2$ | 1.86 | 1.87 | 1.91 | 1.27 | 1.93 | 1.66 | 1.73[3] |

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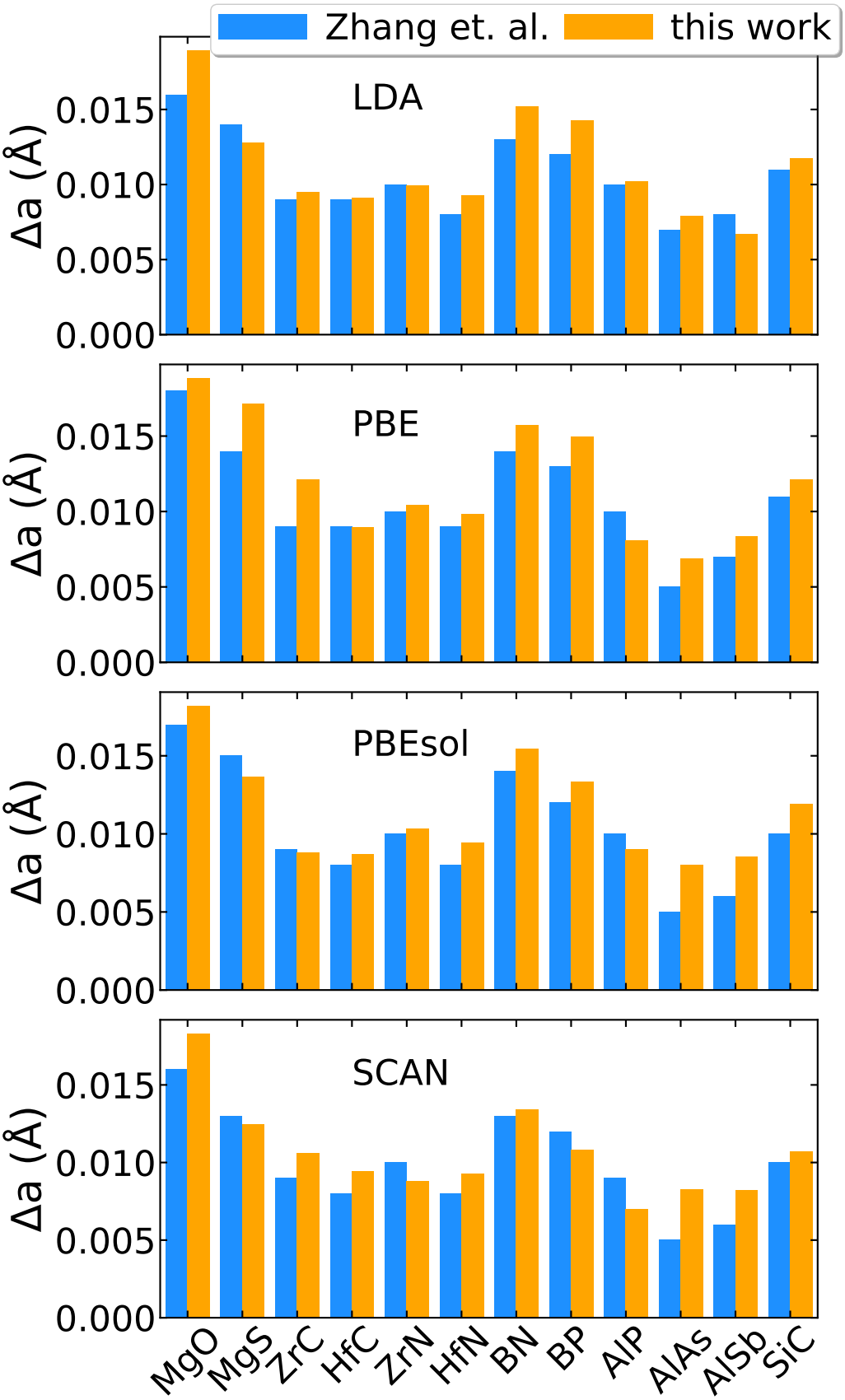


Figure S1: Comparison of the zero-point correction (the difference between the ZPE-corrected lattice constants and non-ZPE-corrected ones) between the previous work (Zhang *et al.* Ref. [4]) and our work (this work) with four different functionals.

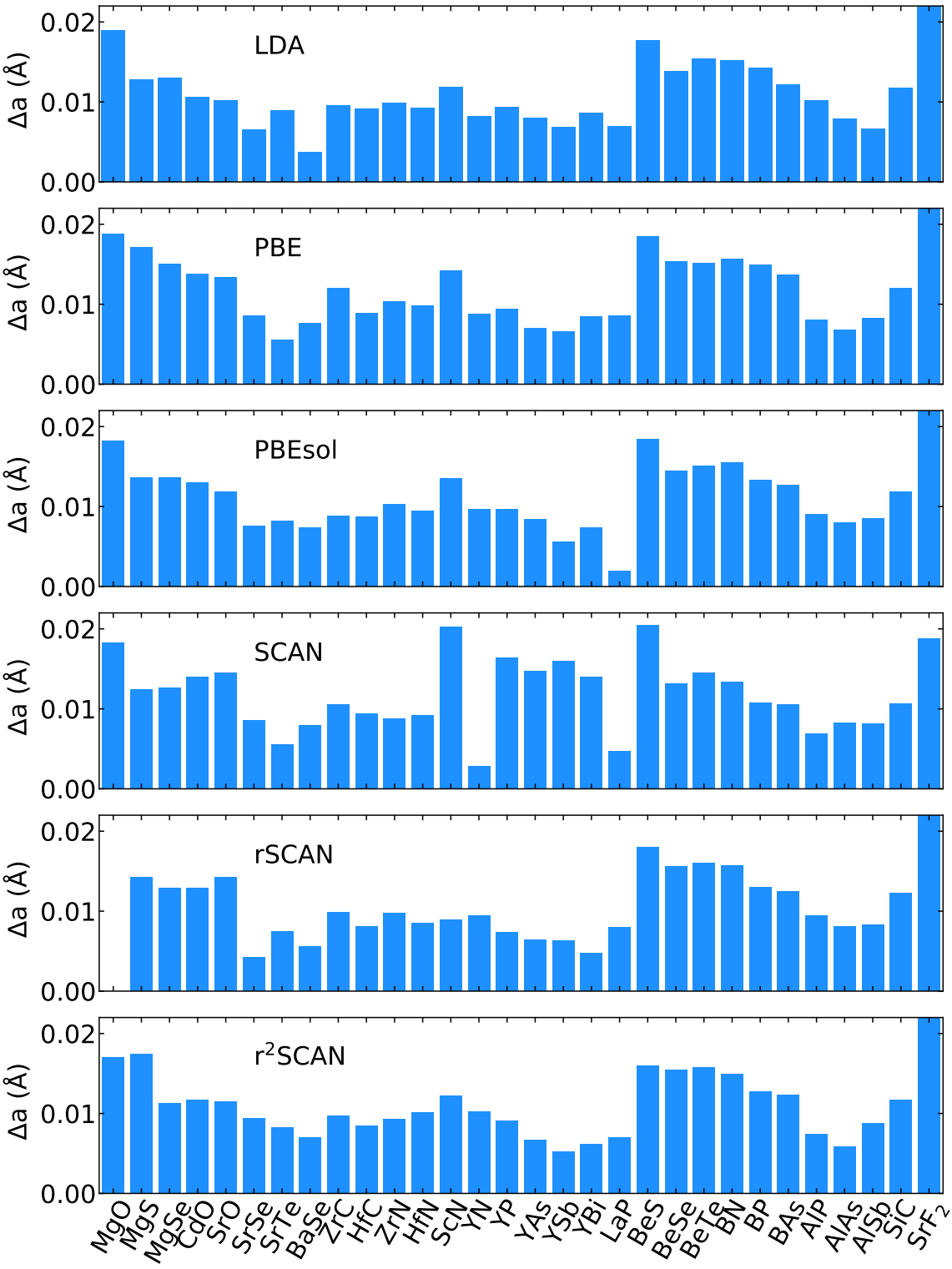


Figure S2: The difference (Δa) between the ZPE-corrected lattice constants and non-ZPE-corrected ones with six functionals used in this work.

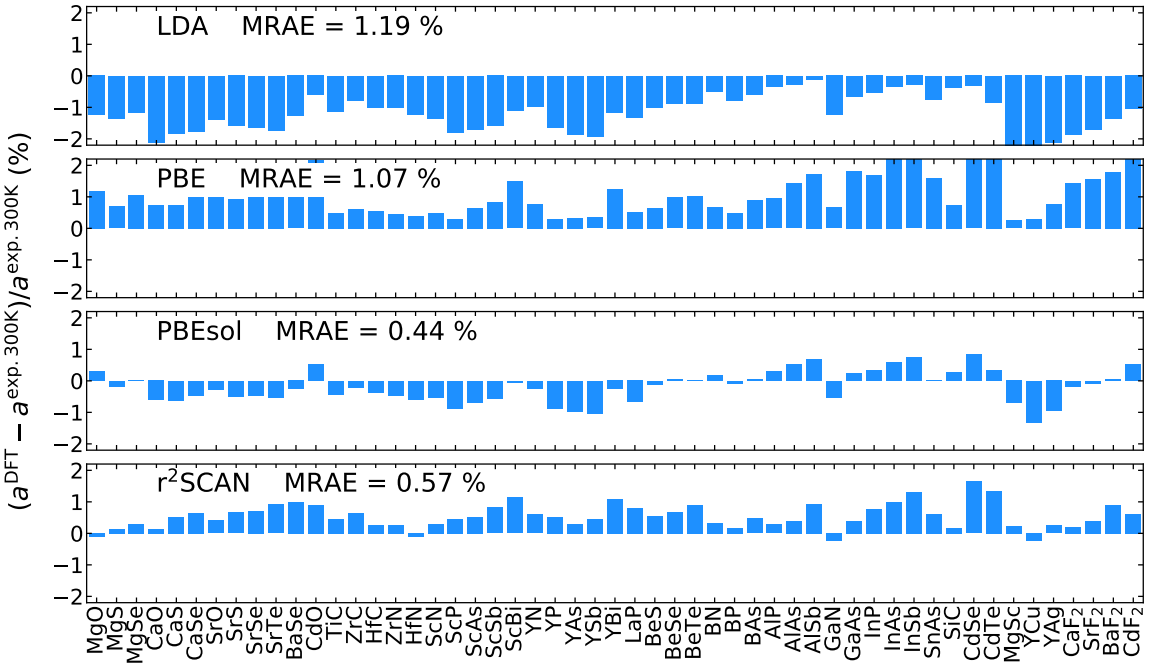


Figure S3: The relative error of lattice constants calculated using different functionals with ZPE correction with respect to experimental values.

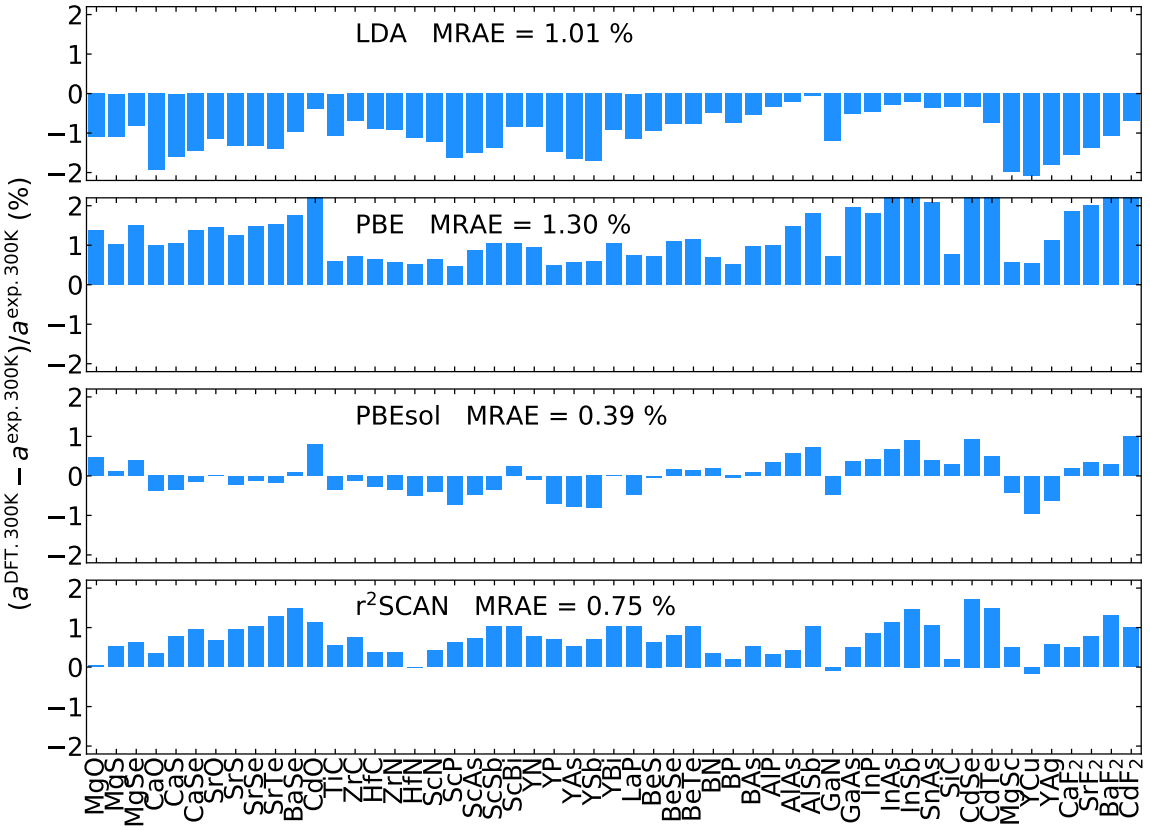


Figure S4: The relative error of DFT calculated lattice constants at 300 K with respect to experimental values at room temperature.

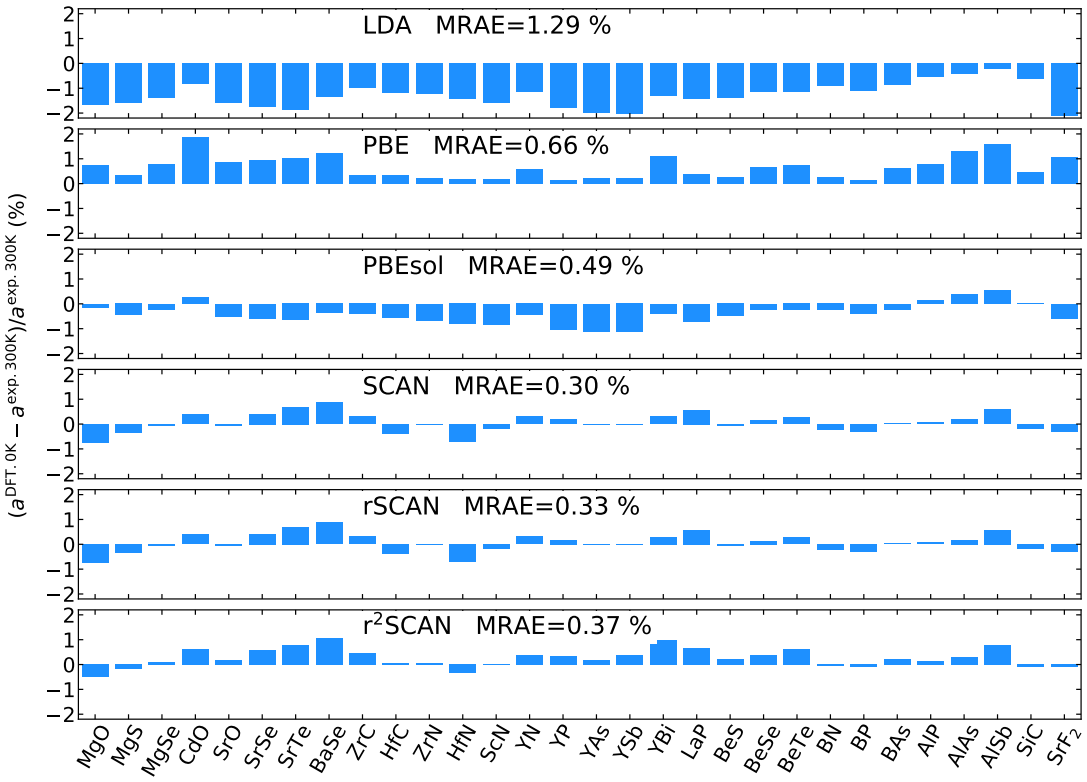


Figure S5: Relative errors of lattice constants computed at 0K with respect to experiment values at room temperature.

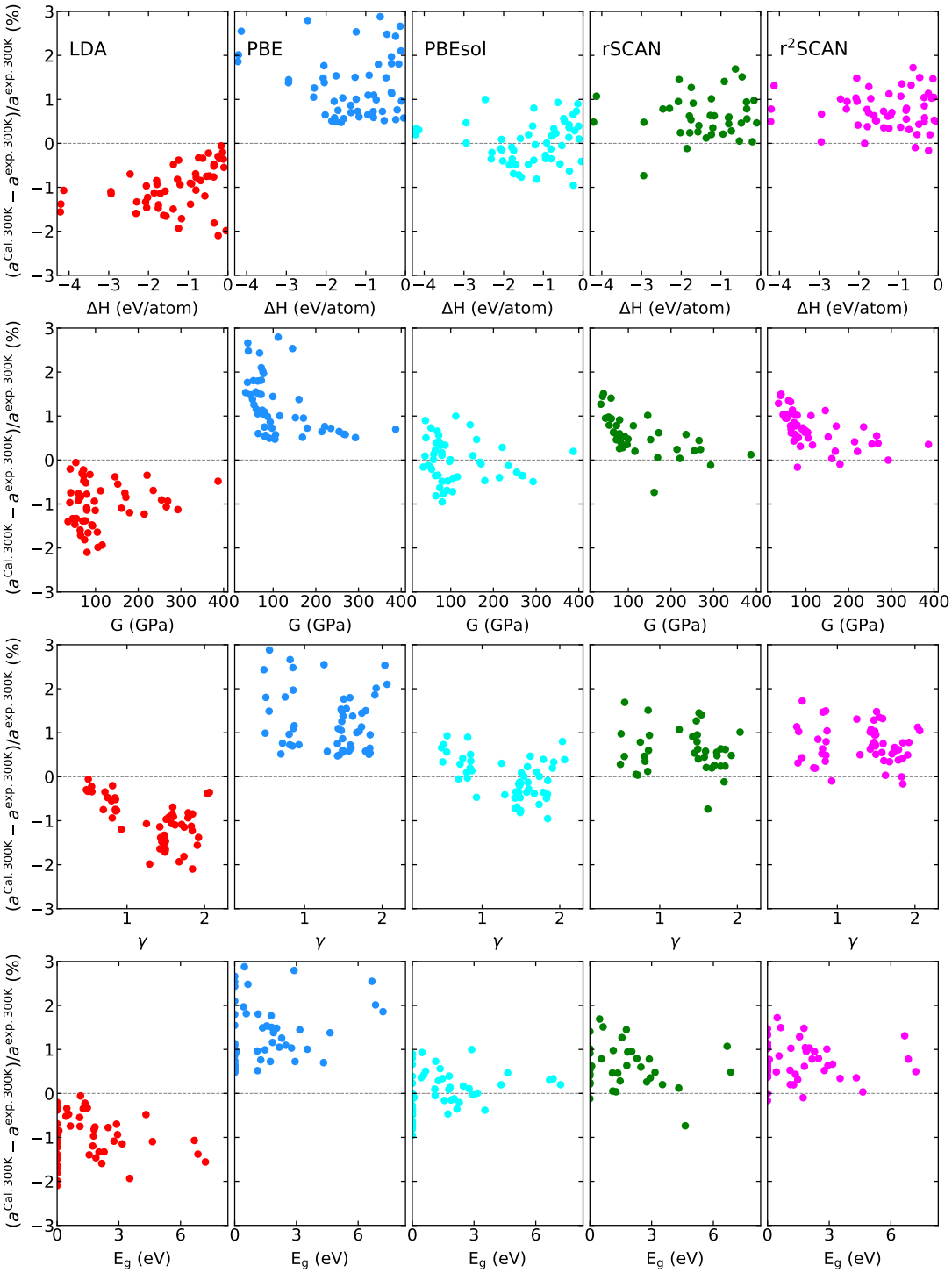


Figure S6: Correlation between the relative errors of DFT calculated lattice constants at 300 K within the QHA with respect to the experimental values at room temperature and formation energy adapted from the OQMD [5], bulk modulus, Grüneisen parameter at room temperature, and band gaps calculated by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

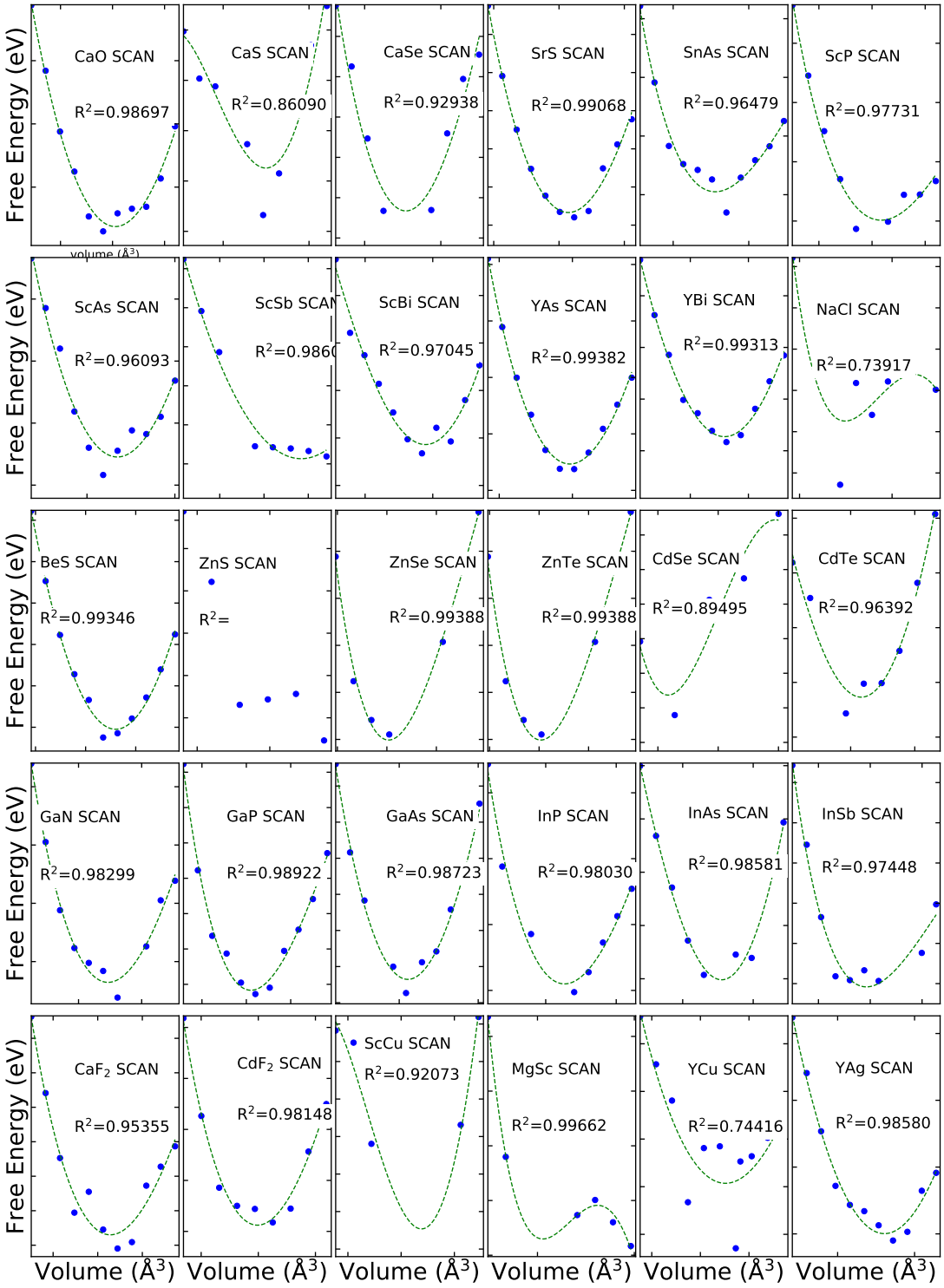


Figure S7: The compounds with poor equation of state fitting ($R^2 \leq 0.995$) for Helmholtz free energy using SCAN.

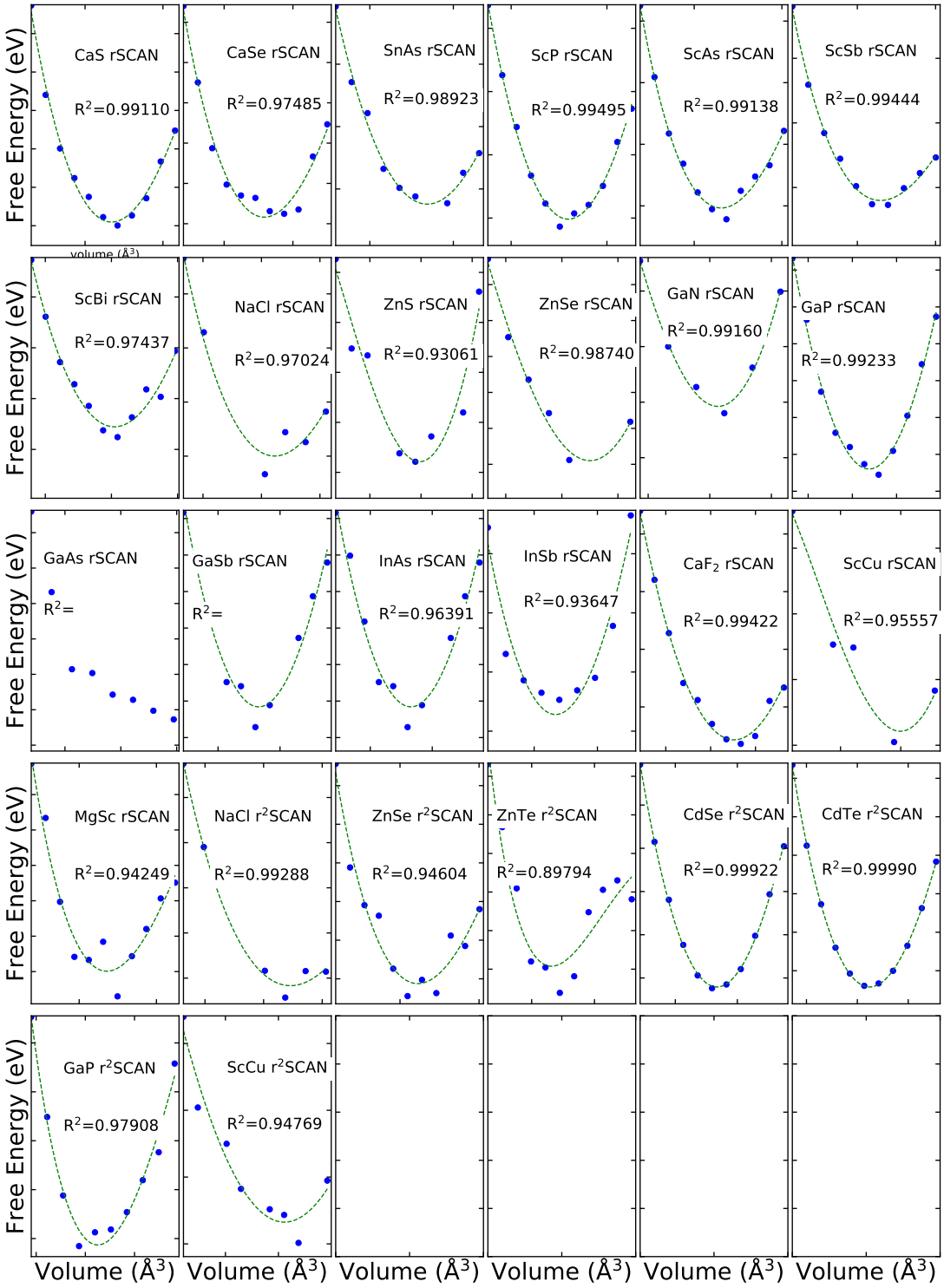


Figure S8: The compounds with poor equation of state fitting ($R^2 \leq 0.995$) for Helmholtz free energy using rSCAN and r$^2$SCAN.

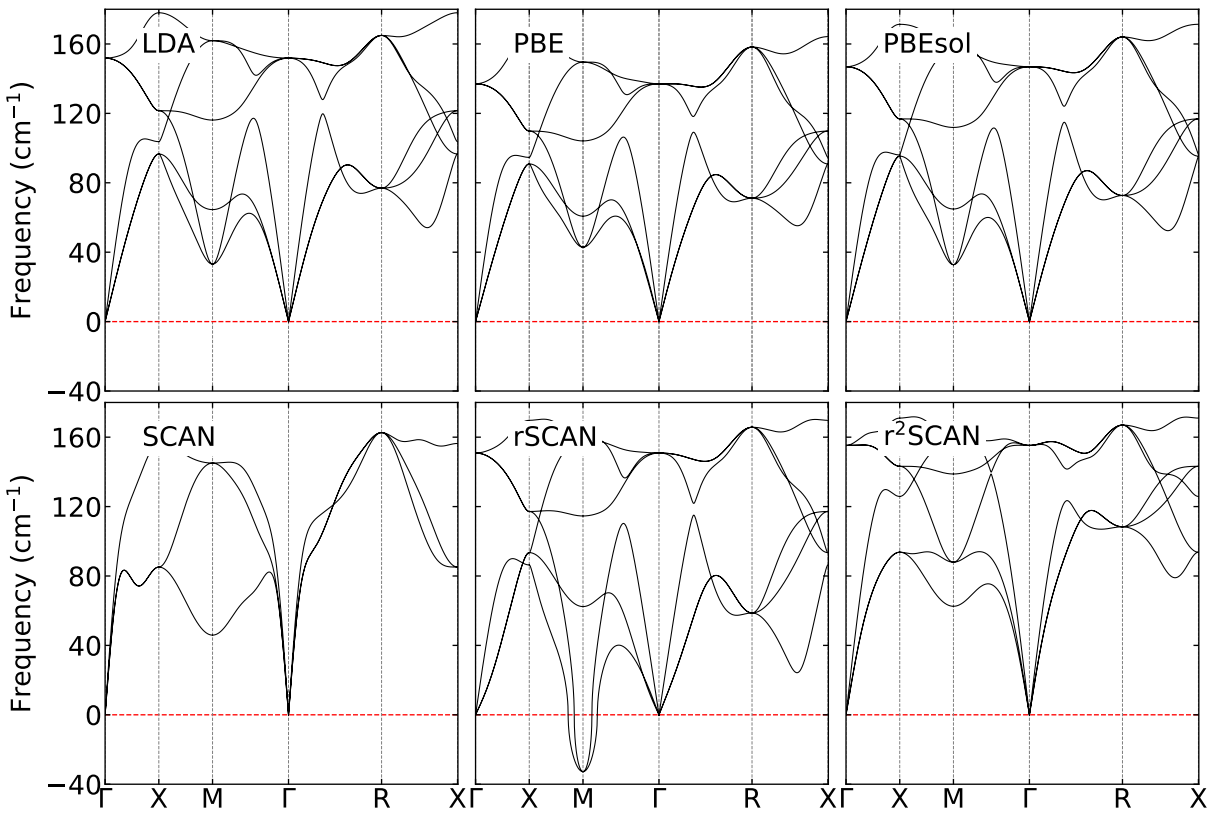


Figure S9: Phonon spectra of YCu calculated by LDA, PBE, PBEsol, SCAN, rSCAN, and r$^2$SCAN. The negative frequency indicates an imaginary frequency.

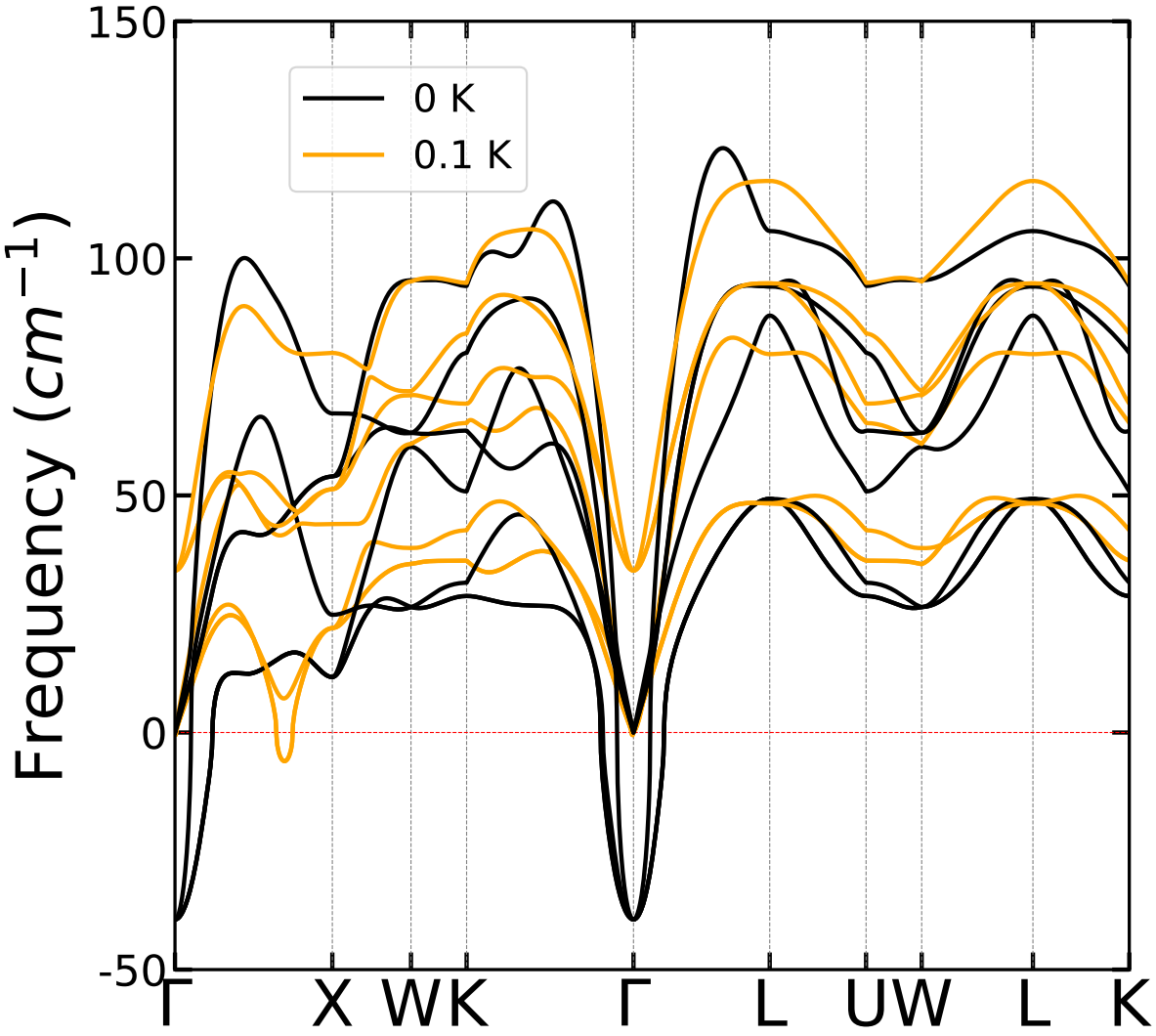


Figure S10: Phonon spectra of PbTe calculated at 0 K and 0.1 K using SCAN functional.