## Supplementary Material

# Performance of various density-functional approximations for cohesive properties of 64 bulk solids

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**Comparison of FHI-aims and WIEN2k EOS calculations**

Now we discuss the reliability of the numerical implementation of DFT approaches in the FHI-aims computational package for bulk crystals. The FHI-aims code offers accurate and efficient implementation of DFT with (semi-)local and hybrid functionals to obtain ground-state properties of periodic and cluster systems (up to systems with thousands of atoms).[1] For periodic solids, the performance of FHI-aims can be seen when comparing the present results with those reported using the WIEN2k code,[2] which is based upon the full-potential linearized augmented plane-wave and local orbitals method to solve the KS equations and is normally regarded as the reference for solid-state studies, as long as numerical accuracy is achieved. The WIEN2k code developers in Blaha's group have carried out extensive tests on cohesive properties of solids using various density functionals. We compare our results with their work. For the same database of 55 solids, excellent agreement is found with the reported WIEN2k values using both the LDA and PBE functionals,[3–5] with the mean absolute deviations of 0.003 Å for the lattice constant and 0.5 GPa for the bulk modulus. In their very recent work, Tran *et al.*[6] have extended assessment to more newly developed functionals. We analyze the mean absolute deviations bewteen the two codes for the cohesive properties of a test set of 40 cubic solids. As shown in table I, we have found that the LDA and PBE results agree closely, followed by PBEsol and SCAN with poorer agreement. For instance, the deviations between the two implementations of PBE are within 0.003 Å for the lattice constant, 33 meV for the cohesive energy, and 0.6 GPa for the bulk modulus. It should be noted that our SCAN calculations were carried out using the PBE orbitals and densities. This is because the functionality to perform SCAN calculations in self-consistent manner is not yet available within the FHI-aims code. Neither does the SCAN implementation in the WIEN2k. While the WIEN2k results are also non-self consistent, they pointed out that the error in the lattice constant induced by this non-self-consistent procedure can be of the order of $\sim$0.02 Å and should be in most cases below 0.005 Å and that the effect on the cohesive energy should be below 50 meV/atom except in the eventual cases where self-consistency would yield a different atomic electronic configuration from the one obtained with PBE for the isolated atom.[6] We have also compared our cohesive properties for SCAN with the reported self-consistent results using the VASP code,[7] with the mean absolute deviations are within 0.007 Å for the lattice constant and 60 meV for the cohesive energy, in agreement with the discussion by Tran *et al.* Though there are other variables (such as basis sets and pseudopotentials) that may amplify differences due to non-self-consistency, both the WIEN2k and our results suggest the post-SCF procedure is an acceptable approximation. Such deviations will not affect the conclusions of the present work, especially as our focus is on the trends in errors and improved methods for describing a wider range of bulk solids and properties in a consistent and efficient way. Further comparison of FHI-aims with WIEN2k can be done based on fully self-consistent calculations of 71 elemental crystals. Lejaeghere and co-authors[8] proposed a method for evaluating numerical errors between different DFT codes and a more close look at the deviations of our results from those of WIEN2k shows remarkably accurate implementation of FHI-aims. Based upon this criterion, a recent benchmarking study from a highly international collaboration demonstrates that a reproducible precision for DFT predictions can be achieved, and they show that FHI-aims is among the most reliable all-electron codes today.[9]

TABLE I. The mean absolute deviations of the lattice constants $a_0$ (Å), the cohesive energies $E_0$ (eV/atom), and the bulk moduli $B_0$ (GPa) between the present work and the reported WIEN2k calculations (taken from Ref. 6) using different DFAs for the dataset of 40 solids.

| Functional | $a_0$ (Å) | $E_0$ (eV/atom) | $B_0$ (GPa) |
|---|---|---|---|
| LDA | 0.003 | 0.023 | 0.9 |
| PBE | 0.003 | 0.033 | 0.6 |
| PBEsol | 0.004 | 0.035 | 1.0 |
| SCAN | 0.005 | 0.048 | 2.4 |

**FHI-aims DFT EOS results**

TABLE II. Equilibrium lattice constants (Å) of 24 metals. The zero-point energy (ZPE) was determined by calculating the phonon dispersion relation at a set of volumes, marked as "Corr.", and "Uncorr." refers as to the non-ZPE-corrected values. Experimental values with ZPE are summarized in the last columns (at 0 K unless noted otherwise).

| Solid | LDA | | PBE | | PBEsol | | M06-L | | SCAN | | HSE06 | | Exp.* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | |
| Li | 3.366 | 3.387 | 3.436 | 3.462 | 3.434 | 3.461 | 3.409 | 3.437 | 3.474 | 3.503 | 3.466 | 3.490 | 3.477 |
| Na | 4.052 | 4.067 | 4.203 | 4.219 | 4.172 | 4.189 | 4.029 | 4.046 | 4.207 | 4.223 | 4.215 | 4.231 | 4.225 |
| K | 5.043 | 5.055 | 5.284 | 5.301 | 5.214 | 5.230 | 4.924 | 4.943 | 5.317 | 5.337 | 5.313 | 5.328 | 5.225 |
| Rb | 5.376 | 5.385 | 5.669 | 5.677 | 5.568 | 5.576 | 5.238 | 5.247 | 5.703 | 5.708 | 5.756 | 5.765 | 5.585 |
| Ca | 5.336 | 5.346 | 5.527 | 5.538 | 5.455 | 5.466 | 5.384 | 5.392 | 5.549 | 5.559 | 5.582 | 5.593 | 5.565 |
| Sr | 5.789 | 5.795 | 6.020 | 6.028 | 5.907 | 5.914 | 5.881 | 5.887 | 6.076 | 6.085 | 6.092 | 6.100 | 6.048 |
| Ba | 4.758 | 4.760 | 5.011 | 5.015 | 4.868 | 4.872 | 4.983 | 4.987 | 5.036 | 5.039 | 5.087 | 5.091 | 5.007 |
| Al | 3.985 | 3.998 | 4.041 | 4.054 | 4.015 | 4.028 | 3.948 | 3.957 | 4.014 | 4.028 | 4.020 | 4.033 | 4.032 |
| Pb | 4.879 | 4.884 | 5.036 | 5.041 | 4.929 | 4.933 | 5.068 | 5.072 | 4.970 | 4.974 | 5.009 | 5.014 | 4.905 |
| Fe | 2.747 | 2.750 | 2.831 | 2.834 | 2.786 | 2.790 | 2.856 | 2.860 | 2.818 | 2.822 | 2.897 | 2.903 | 2.861 |
| V | 2.924 | 2.929 | 2.996 | 3.001 | 2.957 | 2.962 | 2.997 | 3.001 | 2.971 | 2.975 | 2.970 | 2.974 | 3.028 |
| Mo | 3.111 | 3.114 | 3.161 | 3.164 | 3.130 | 3.132 | 3.163 | 3.166 | 3.143 | 3.146 | 3.145 | 3.147 | 3.144 |
| W | 3.134 | 3.136 | 3.183 | 3.185 | 3.153 | 3.155 | 3.184 | 3.186 | 3.150 | 3.152 | 3.173 | 3.175 | 3.162 |
| Nb | 3.247 | 3.250 | 3.310 | 3.313 | 3.271 | 3.274 | 3.322 | 3.325 | 3.294 | 3.297 | 3.305 | 3.308 | 3.296 |
| Ta | 3.250 | 3.253 | 3.318 | 3.320 | 3.278 | 3.280 | 3.328 | 3.330 | 3.274 | 3.276 | 3.328 | 3.330 | 3.301 |
| Ni | 3.423 | 3.429 | 3.518 | 3.524 | 3.462 | 3.468 | 3.492 | 3.499 | 3.458 | 3.465 | 3.512 | 3.519 | 3.513 |
| Cu | 3.521 | 3.527 | 3.631 | 3.638 | 3.564 | 3.571 | 3.597 | 3.604 | 3.558 | 3.565 | 3.633 | 3.640 | 3.603 |
| Rh | 3.754 | 3.758 | 3.830 | 3.834 | 3.779 | 3.783 | 3.822 | 3.826 | 3.785 | 3.789 | 3.797 | 3.801 | 3.798 |
| Ir | 3.813 | 3.815 | 3.870 | 3.872 | 3.829 | 3.831 | 3.856 | 3.859 | 3.814 | 3.816 | 3.840 | 3.843 | 3.835 |
| Pd | 3.842 | 3.846 | 3.942 | 3.947 | 3.873 | 3.878 | 3.939 | 3.944 | 3.890 | 3.895 | 3.929 | 3.934 | 3.881 |
| Pt | 3.895 | 3.897 | 3.970 | 3.973 | 3.917 | 3.920 | 3.959 | 3.962 | 3.910 | 3.913 | 3.949 | 3.952 | 3.916 |
| Ag | 4.004 | 4.009 | 4.149 | 4.155 | 4.052 | 4.058 | 4.159 | 4.165 | 4.083 | 4.088 | 4.153 | 4.159 | 4.069 |
| Au | 4.054 | 4.058 | 4.157 | 4.161 | 4.081 | 4.084 | 4.158 | 4.163 | 4.094 | 4.098 | 4.153 | 4.157 | 4.065 |
| Th | 4.885 | 4.887 | 5.033 | 5.036 | 4.926 | 4.929 | 5.119 | 5.121 | 4.933 | 4.936 | 5.110 | 5.112 | 5.074 |

* Li(20 K)[10], Na(5 K)[11], K(5 K)[11], Rb(5 K)[11], Ca[12], Sr[12], Ba[12], Al[13], Pb(5 K)[14,15], Fe[4,5], V[4,5], Mo[4,5], W[4,5], Nb[4,5], Ta[4,5], Ni(10 K)[15,16], Cu[17,18], Rh[17,18], Ir(5 K)[14], Pd[17,18], Pt[4,5], Au(5 K)[14], Ag[17,18], Th[4,5].

TABLE III. Equilibrium lattice constants (Å) of 40 non-metallic solids.

| Solid | LDA | | PBE | | PBEsol | | M06-L | | SCAN | | HSE06 | | Exp.* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | |
| LiF | 3.913 | 3.944 | 4.066 | 4.103 | 4.005 | 4.042 | 3.971 | 4.008 | 3.971 | 4.003 | 4.003 | 4.040 | 4.010 |
| LiCl | 4.966 | 4.994 | 5.151 | 5.185 | 5.064 | 5.094 | 5.117 | 5.149 | 5.109 | 5.138 | 5.107 | 5.138 | 5.106 |
| NaF | 4.504 | 4.528 | 4.700 | 4.727 | 4.625 | 4.652 | 4.576 | 4.601 | 4.574 | 4.598 | 4.635 | 4.661 | 4.609 |
| NaCl | 5.469 | 5.491 | 5.698 | 5.721 | 5.600 | 5.624 | 5.575 | 5.598 | 5.585 | 5.607 | 5.645 | 5.667 | 5.595 |
| MgO | 4.164 | 4.180 | 4.254 | 4.272 | 4.214 | 4.231 | 4.200 | 4.216 | 4.194 | 4.210 | 4.208 | 4.224 | 4.207 |
| MgS | 5.139 | 5.153 | 5.231 | 5.245 | 5.182 | 5.197 | 5.179 | 5.193 | 5.195 | 5.208 | 5.207 | 5.221 | 5.202 |
| TiC | 4.261 | 4.271 | 4.333 | 4.345 | 4.293 | 4.304 | 4.311 | 4.322 | 4.319 | 4.329 | 4.307 | 4.318 | 4.330 |
| ZrC | 4.642 | 4.651 | 4.710 | 4.719 | 4.669 | 4.678 | 4.707 | 4.716 | 4.703 | 4.712 | 4.700 | 4.708 | 4.696 |
| HfC | 4.573 | 4.582 | 4.653 | 4.662 | 4.611 | 4.619 | 4.645 | 4.654 | 4.620 | 4.628 | 4.647 | 4.655 | 4.638 |
| VC | 4.088 | 4.099 | 4.156 | 4.167 | 4.117 | 4.128 | 4.119 | 4.131 | 4.134 | 4.145 | 4.112 | 4.123 | 4.160 |
| NbC | 4.427 | 4.434 | 4.486 | 4.495 | 4.450 | 4.458 | 4.462 | 4.470 | 4.473 | 4.481 | 4.461 | 4.469 | 4.470 |
| TiN | 4.172 | 4.182 | 4.247 | 4.258 | 4.204 | 4.214 | 4.247 | 4.258 | 4.225 | 4.235 | 4.213 | 4.223 | 4.239 |
| ZrN | 4.525 | 4.535 | 4.595 | 4.605 | 4.553 | 4.563 | 4.615 | 4.625 | 4.580 | 4.590 | 4.575 | 4.584 | 4.585 |
| HfN | 4.469 | 4.477 | 4.550 | 4.559 | 4.504 | 4.512 | 4.566 | 4.575 | 4.508 | 4.516 | 4.531 | 4.539 | 4.519 |
| VN | 4.042 | 4.051 | 4.117 | 4.130 | 4.073 | 4.083 | 4.111 | 4.124 | 4.091 | 4.102 | 4.073 | 4.083 | 4.135 |
| NbN | 4.356 | 4.362 | 4.421 | 4.429 | 4.380 | 4.386 | 4.424 | 4.431 | 4.403 | 4.409 | 4.392 | 4.398 | 4.379 |
| C | 3.532 | 3.545 | 3.572 | 3.586 | 3.555 | 3.568 | 3.551 | 3.564 | 3.551 | 3.564 | 3.549 | 3.561 | 3.567 |
| Si | 5.405 | 5.414 | 5.470 | 5.479 | 5.431 | 5.440 | 5.425 | 5.434 | 5.433 | 5.442 | 5.444 | 5.452 | 5.430 |
| Ge | 5.625 | 5.630 | 5.761 | 5.767 | 5.664 | 5.669 | 5.787 | 5.795 | 5.669 | 5.674 | 5.702 | 5.709 | 5.652 |
| Sn | 6.474 | 6.480 | 6.651 | 6.659 | 6.527 | 6.534 | 6.718 | 6.726 | 6.550 | 6.558 | 6.580 | 6.588 | 6.482 |
| AlP | 5.434 | 5.444 | 5.508 | 5.518 | 5.470 | 5.480 | 5.457 | 5.466 | 5.475 | 5.484 | 5.482 | 5.491 | 5.458 |
| AlAs | 5.630 | 5.637 | 5.730 | 5.735 | 5.675 | 5.680 | 5.711 | 5.716 | 5.675 | 5.680 | 5.694 | 5.698 | 5.652 |
| AlSb | 6.108 | 6.116 | 6.224 | 6.231 | 6.153 | 6.159 | 6.221 | 6.227 | 6.166 | 6.172 | 6.184 | 6.191 | 6.128 |
| BN | 3.582 | 3.595 | 3.626 | 3.640 | 3.607 | 3.621 | 3.603 | 3.616 | 3.605 | 3.618 | 3.601 | 3.614 | 3.607 |
| BP | 4.492 | 4.504 | 4.549 | 4.562 | 4.521 | 4.533 | 4.519 | 4.532 | 4.528 | 4.540 | 4.530 | 4.542 | 4.538 |
| BAs | 4.733 | 4.744 | 4.810 | 4.822 | 4.768 | 4.779 | 4.792 | 4.804 | 4.772 | 4.783 | 4.781 | 4.792 | 4.777 |
| GaN | 4.460 | 4.469 | 4.548 | 4.559 | 4.498 | 4.508 | 4.539 | 4.549 | 4.494 | 4.504 | 4.504 | 4.513 | 4.520 |
| GaP | 5.398 | 5.406 | 5.507 | 5.515 | 5.437 | 5.445 | 5.501 | 5.509 | 5.444 | 5.452 | 5.467 | 5.475 | 5.442 |
| GaAs | 5.607 | 5.612 | 5.747 | 5.753 | 5.659 | 5.665 | 5.772 | 5.778 | 5.656 | 5.662 | 5.692 | 5.697 | 5.641 |
| GaSb | 6.052 | 6.058 | 6.216 | 6.222 | 6.113 | 6.119 | 6.262 | 6.268 | 6.116 | 6.122 | 6.152 | 6.158 | 6.082 |
| InP | 5.828 | 5.835 | 5.960 | 5.969 | 5.876 | 5.884 | 5.961 | 5.969 | 5.894 | 5.903 | 5.907 | 5.914 | 5.861 |
| InAs | 6.027 | 6.033 | 6.186 | 6.192 | 6.082 | 6.088 | 6.232 | 6.238 | 6.093 | 6.099 | 6.125 | 6.131 | 6.036 |
| InSb | 6.451 | 6.454 | 6.633 | 6.641 | 6.510 | 6.515 | 6.700 | 6.708 | 6.524 | 6.530 | 6.561 | 6.568 | 6.469 |
| SiC | 4.330 | 4.341 | 4.381 | 4.392 | 4.358 | 4.368 | 4.328 | 4.340 | 4.353 | 4.363 | 4.353 | 4.363 | 4.358 |
| ZnS | 5.299 | 5.308 | 5.445 | 5.457 | 5.357 | 5.367 | 5.454 | 5.464 | 5.376 | 5.386 | 5.419 | 5.429 | 5.404 |
| ZnSe | 5.569 | 5.575 | 5.734 | 5.741 | 5.633 | 5.639 | 5.765 | 5.773 | 5.650 | 5.656 | 5.700 | 5.706 | 5.668 |
| ZnTe | 5.997 | 6.004 | 6.180 | 6.194 | 6.063 | 6.070 | 6.239 | 6.246 | 6.084 | 6.090 | 6.152 | 6.159 | 6.104 |
| CdS | 5.761 | 5.768 | 5.929 | 5.939 | 5.825 | 5.833 | 5.948 | 5.957 | 5.860 | 5.869 | 5.885 | 5.894 | 5.818 |
| CdSe | 6.011 | 6.017 | 6.197 | 6.203 | 6.080 | 6.085 | 6.247 | 6.253 | 6.114 | 6.119 | 6.147 | 6.152 | 6.050 |
| CdTe | 6.412 | 6.418 | 6.620 | 6.627 | 6.487 | 6.492 | 6.696 | 6.703 | 6.523 | 6.530 | 6.574 | 6.579 | 6.480 |

* LiF[13], LiCl[13], NaF[13], NaCl[13], MgO[13], MgS[19,20], TiC[21,22], ZrC[21,22], HfC[21,22], VC[21–23], NbC[21,22], TiN[21,22], ZrN[21,22], HfN[21,22], VN[24,25], NbN[22,26], C[27], Si[28], Ge[28], Sn(20 K)[29,30], SiC[14,17], AlP[31], AlAs[31], AlSb[31], BN[29], BP[29], BAs[32], GaN[30], GaP[31], GaAs[31], GaSb[31], InP[31], InAs[31], InSb[31], ZnS(4.2 K)[33], ZnSe[29,34], ZnTe[35], CdS[36], CdSe[37], CdTe[37].

TABLE IV. Equilibrium bulk moduli (GPa) of 24 metals

| Solid | LDA | | PBE | | PBEsol | | M06-L | | SCAN | | HSE06 | | Exp.* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | |
| Li | 15.2 | 14.2 | 14.1 | 13.5 | 13.7 | 12.9 | 12.5 | 11.5 | 11.2 | 12.5 | 13.7 | 13.3 | 12.8 |
| Na | 9.1 | 8.9 | 7.7 | 7.5 | 7.7 | 7.6 | 8.4 | 7.9 | 8.0 | 7.9 | 7.8 | 7.6 | 7.5 |
| K | 4.5 | 4.7 | 3.6 | 3.57 | 3.8 | 3.4 | 5.3 | 5.6 | 3.4 | 3.7 | 3.4 | 3.4 | 3.7 |
| Rb | 3.6 | 3.6 | 2.8 | 2.79 | 3.0 | 2.9 | 5.0 | 5.0 | 2.9 | 3.2 | 2.5 | 2.5 | 3.1 |
| Ca | 18.8 | 18.5 | 17.4 | 17.1 | 17.9 | 17.6 | 22.0 | 21.6 | 18.3 | 18.2 | 17.2 | 17.3 | 18.4 |
| Sr | 14.3 | 14.3 | 11.5 | 11.4 | 12.7 | 12.6 | 17.0 | 16.8 | 10.7 | 10.6 | 11.3 | 11.2 | 12.4 |
| Ba | 10.3 | 10.2 | 8.8 | 8.8 | 8.8 | 8.0 | 11.8 | 11.8 | 8.8 | 8.8 | 8.4 | 8.4 | 9.3 |
| Al | 83.7 | 81.3 | 77.6 | 76.0 | 82.3 | 80.8 | 117.0 | 116.2 | 80.4 | 78.7 | 82.9 | 82.0 | 79.4 |
| Pb | 53.7 | 52.6 | 40.0 | 39.6 | 48.8 | 48.6 | 38.8 | 38.8 | 46.4 | 45.9 | 43.6 | 43.3 | 48.8 |
| Fe | 252.1 | 252.7 | 195.1 | 190.2 | 227.6 | 229.5 | 152.0 | 145.4 | 185.3 | 185.3 | 150.9 | 145.1 | 173.0 |
| V | 209.1 | 207.0 | 182.6 | 180.8 | 197.5 | 197.5 | 192.6 | 192.8 | 197.6 | 197.9 | 212.4 | 211.9 | 157.0 |
| Mo | 293.0 | 290.2 | 259.1 | 256.5 | 279.0 | 276.0 | 266.8 | 264.3 | 278.8 | 275.9 | 285.5 | 282.9 | 265.3 |
| W | 335.9 | 334.3 | 301.9 | 300.3 | 321.5 | 319.7 | 319.9 | 318.6 | 325.6 | 323.8 | 329.9 | 328.5 | 314.2 |
| Nb | 195.2 | 192.4 | 169.7 | 167.5 | 180.5 | 179.1 | 174.2 | 173.2 | 177.7 | 176.5 | 184.0 | 182.4 | 174.0 |
| Ta | 211.9 | 210.5 | 194.1 | 193.3 | 206.4 | 206.4 | 202.1 | 201.5 | 205.5 | 205.5 | 221.9 | 221.1 | 194.2 |
| Ni | 256.7 | 251.6 | 199.4 | 196.3 | 231.2 | 228.3 | 217.8 | 215.9 | 231.8 | 228.1 | 190.0 | 185.4 | 187.6 |
| Cu | 187.3 | 184.1 | 139.4 | 136.8 | 165.3 | 162.3 | 154.8 | 152.2 | 168.4 | 165.5 | 130.7 | 127.9 | 142.3 |
| Rh | 317.8 | 315.0 | 257.1 | 254.2 | 294.5 | 291.9 | 263.3 | 261.3 | 293.7 | 291.2 | 281.6 | 279.0 | 268.7 |
| Ir | 403.4 | 400.8 | 350.1 | 347.4 | 393.1 | 390.5 | 370.6 | 367.9 | 411.1 | 409.1 | 383.3 | 380.7 | 383.0 |
| Pd | 226.9 | 224.2 | 168.6 | 166.2 | 203.2 | 200.5 | 165.9 | 163.0 | 195.0 | 192.2 | 169.7 | 167.0 | 195.0 |
| Pt | 307.4 | 305.3 | 249.1 | 246.9 | 289.8 | 287.9 | 259.6 | 257.3 | 294.3 | 292.5 | 262.8 | 260.7 | 277.0 |
| Ag | 138.7 | 135.6 | 91.0 | 89.3 | 118.5 | 116.9 | 88.4 | 87.1 | 110.2 | 108.3 | 88.7 | 87.3 | 110.9 |
| Au | 194.6 | 192.8 | 139.7 | 137.7 | 176.5 | 174.2 | 135.1 | 133.5 | 168.3 | 166.1 | 141.6 | 140.2 | 180.9 |
| Th | 63.3 | 63.8 | 55.2 | 55.1 | 60.4 | 60.1 | 55.0 | 54.1 | 56.7 | 56.3 | 54.4 | 53.8 | 57.7 |

* Li[38], Na[39], K[40], Rb[41], Ca[12], Sr[12], Ba[12], Al[42], Pb[43], Fe[44,45], V[46], Mo[47], W[47], Nb[48–50], Ta[47], Ni[44,45], Cu[51,52], Rh(4.2 K)[53], Ir[54], Pd[55], Pt[56,57], Au[52], Ag[52], Th[57,58].

TABLE V. Equilibrium bulk moduli (GPa) of 40 non-metallic solids

| Solid | LDA | | PBE | | PBEsol | | M06-L | | SCAN | | HSE06 | | Exp.* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | |
| LiF | 85.4 | 79.2 | 67.2 | 61.6 | 72.8 | 69.3 | 76.8 | 70.6 | 86.6 | 79.2 | 77.9 | 72.3 | 69.8 |
| LiCl | 40.8 | 39.7 | 31.7 | 29.8 | 35.0 | 32.6 | 35.0 | 32.2 | 36.3 | 35.3 | 35.1 | 32.8 | 35.4 |
| NaF | 61.7 | 58.8 | 45.3 | 42.6 | 49.1 | 46.9 | 53.7 | 51.2 | 56.4 | 53.9 | 49.2 | 48.3 | 51.4 |
| NaCl | 32.2 | 31.3 | 23.7 | 23.0 | 26.0 | 25.8 | 27.1 | 26.2 | 28.7 | 28.7 | 25.3 | 24.1 | 28.5 |
| MgO | 171.7 | 166.9 | 149.4 | 145.2 | 157.7 | 153.0 | 165.3 | 159.8 | 169.6 | 164.9 | 165.0 | 160.5 | 168.8 |
| MgS | 82.8 | 81.0 | 73.8 | 71.7 | 78.0 | 76.9 | 81.5 | 80.4 | 80.1 | 79.1 | 78.8 | 77.8 | 78.9 |
| TiC | 282.6 | 277.1 | 249.6 | 244.1 | 266.0 | 259.7 | 267.7 | 261.9 | 268.5 | 263.7 | 276.8 | 271.2 | 244.0 |
| ZrC | 246.6 | 242.5 | 222.0 | 218.1 | 235.1 | 231.7 | 230.0 | 226.2 | 231.4 | 228.1 | 237.0 | 234.0 | 226.0 |
| HfC | 260.2 | 255.2 | 236.5 | 233.6 | 250.2 | 247.4 | 249.2 | 246.6 | 254.0 | 250.6 | 248.2 | 245.3 | 275.0 |
| VC | 346.8 | 341.3 | 306.2 | 301.5 | 329.4 | 328.5 | 329.8 | 328.4 | 330.3 | 329.0 | 347.8 | 347.8 | 303.0 |
| NbC | 333.4 | 324.5 | 299.4 | 289.1 | 318.3 | 308.8 | 315.6 | 306.1 | 313.6 | 304.3 | 327.1 | 317.7 | 302.0 |
| TiN | 320.7 | 313.9 | 278.0 | 271.5 | 301.4 | 295.6 | 284.6 | 279.3 | 301.4 | 294.5 | 311.6 | 305.9 | 289.0 |
| ZrN | 283.7 | 277.8 | 250.3 | 245.0 | 276.6 | 270.9 | 244.8 | 240.4 | 265.8 | 260.9 | 269.8 | 265.0 | 215.0 |
| HfN | 301.7 | 296.1 | 260.8 | 254.5 | 277.5 | 272.8 | 257.7 | 251.5 | 284.6 | 280.8 | 283.8 | 280.5 | 306.0 |
| VN | 367.2 | 353.3 | 314.9 | 301.6 | 344.5 | 325.3 | 317.2 | 298.6 | 342.2 | 322.7 | 356.8 | 335.9 | 268.0 |
| NbN | 351.0 | 345.4 | 306.9 | 298.4 | 332.8 | 324.5 | 303.8 | 295.7 | 326.8 | 318.7 | 339.0 | 330.7 | 292.0 |
| C | 467.0 | 456.8 | 434.3 | 424.0 | 451.2 | 435.2 | 452.8 | 437.8 | 459.6 | 445.0 | 468.8 | 452.9 | 443.0 |
| Si | 96.2 | 94.6 | 88.6 | 87.5 | 95.3 | 94.8 | 97.7 | 97.5 | 99.1 | 99.0 | 97.6 | 97.4 | 99.2 |
| Ge | 72.4 | 70.2 | 59.4 | 57.3 | 66.9 | 66.0 | 58.3 | 56.5 | 72.2 | 71.3 | 70.2 | 67.9 | 75.8 |
| Sn | 44.9 | 43.8 | 35.9 | 35.4 | 41.4 | 39.4 | 35.0 | 34.8 | 41.8 | 40.7 | 43.2 | 42.8 | 53.0 |
| AlP | 89.4 | 87.4 | 82.4 | 81.4 | 86.6 | 84.6 | 91.1 | 89.1 | 89.5 | 87.4 | 94.5 | 91.6 | 86.0 |
| AlAs | 75.0 | 74.2 | 66.9 | 65.7 | 71.8 | 71.9 | 70.4 | 69.4 | 75.8 | 76.3 | 74.5 | 74.1 | 78.1 |
| AlSb | 56.0 | 55.8 | 49.2 | 49.0 | 54.3 | 55.0 | 51.6 | 51.7 | 56.3 | 56.7 | 55.2 | 54.5 | 59.3 |
| BN | 402.1 | 392.8 | 374.1 | 363.6 | 388.0 | 373.8 | 391.7 | 380.8 | 394.5 | 379.6 | 399.6 | 389.8 | 378.0 |
| BP | 175.2 | 171.5 | 162.0 | 158.5 | 169.5 | 165.9 | 170.1 | 166.5 | 171.1 | 168.9 | 173.0 | 169.7 | 173.0 |
| AsB | 146.6 | 143.8 | 131.7 | 128.7 | 140.8 | 138.4 | 134.2 | 131.6 | 145.6 | 143.1 | 143.3 | 140.4 | 148.0 |
| GaN | 201.6 | 197.7 | 172.0 | 168.0 | 188.9 | 184.9 | 179.6 | 176.0 | 193.7 | 189.5 | 197.4 | 193.3 | 200.0 |
| GaP | 89.1 | 87.4 | 76.6 | 75.5 | 85.1 | 83.7 | 81.1 | 79.5 | 88.0 | 86.7 | 87.9 | 86.4 | 88.7 |
| GaAs | 74.2 | 74.0 | 60.7 | 59.5 | 69.0 | 69.0 | 61.5 | 60.3 | 72.4 | 72.5 | 70.9 | 70.0 | 76.9 |
| GaSb | 55.5 | 55.1 | 44.5 | 44.0 | 52.0 | 51.8 | 44.0 | 43.7 | 53.6 | 53.4 | 53.0 | 52.7 | 56.3 |
| InP | 70.8 | 68.6 | 59.9 | 58.9 | 67.1 | 65.6 | 63.6 | 62.6 | 69.3 | 68.1 | 69.4 | 68.4 | 72.5 |
| InAs | 59.9 | 59.1 | 48.1 | 47.7 | 56.4 | 56.5 | 47.6 | 47.1 | 58.1 | 57.9 | 57.2 | 56.8 | 58.0 |
| InSb | 46.5 | 44.0 | 36.9 | 36.2 | 44.1 | 43.3 | 36.3 | 35.8 | 44.5 | 43.5 | 44.0 | 42.7 | 46.5 |
| SiC | 228.7 | 225.2 | 212.9 | 209.0 | 222.0 | 220.9 | 225.1 | 221.6 | 229.9 | 227.4 | 228.9 | 225.4 | 225.0 |
| ZnS | 86.4 | 84.6 | 69.7 | 68.8 | 79.0 | 76.5 | 74.6 | 74.1 | 79.9 | 77.6 | 77.0 | 75.9 | 77.2 |
| ZnSe | 71.5 | 71.4 | 56.7 | 55.5 | 65.3 | 64.5 | 58.2 | 57.2 | 66.1 | 65.1 | 63.3 | 61.9 | 64.7 |
| ZnTe | 55.4 | 54.9 | 43.3 | 43.0 | 50.5 | 50.6 | 42.1 | 42.8 | 50.6 | 49.8 | 48.9 | 48.6 | 52.8 |
| CdS | 68.0 | 64.3 | 53.5 | 52.8 | 61.5 | 59.8 | 57.7 | 56.7 | 61.5 | 60.1 | 60.8 | 59.3 | 64.3 |
| CdSe | 58.0 | 57.9 | 44.8 | 44.3 | 52.6 | 52.4 | 46.1 | 45.6 | 52.6 | 52.1 | 51.2 | 50.3 | 55.0 |
| CdTe | 46.2 | 48.2 | 35.2 | 33.5 | 41.6 | 40.1 | 35.2 | 34.8 | 41.3 | 39.3 | 40.1 | 39.4 | 44.5 |

* LiF[59], LiCl[60], NaF[60], NaCl[61], MgO[62], MgS[19], TiC[63], ZrC[63], HfC (296 K)[64,65], VC[66], NbC[67,68], TiN[69], ZrN(300 K)[26], HfN(300 K)[26], VN(300 K)[70], NbN(300 K)[26], C[17,18], Si(77 K)[71], Ge(4.2 K)[72], Sn(90 K)[73,74], SiC[75], AlP[13,76], AlAs[76,77], AlSb[76,77], BN[78], BP[79], BAs[32], GaN[13], GaP[76,77], GaAs[80], GaSb[76,77], InP[76,77], InAs[76,77], InSb[76,77], ZnS[81], ZnSe[81], ZnTe[81], CdS[37], CdSe[37], CdTe[81].

TABLE VI. Equilibrium cohesive energies (eV/atom) of 24 metals. The experimental values are taken from Ref. 82 at 0 K.

| Solid | LDA | | PBE | | PBEsol | | M06-L | | SCAN | | HSE06 | | Exp. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | |
| Li | −1.80 | −1.76 | −1.68 | −1.64 | −1.75 | −1.71 | −1.88 | −1.85 | −1.60 | −1.57 | −1.62 | −1.59 | −1.63 |
| Na | −1.25 | −1.23 | −1.10 | −1.08 | −1.17 | −1.15 | −1.45 | −1.43 | −1.08 | −1.06 | −1.06 | −1.04 | −1.11 |
| K | −1.03 | −1.02 | −0.88 | −0.88 | −0.95 | −0.94 | −1.35 | −1.34 | −0.85 | −0.84 | −0.85 | −0.84 | −0.93 |
| Rb | −0.94 | −0.93 | −0.79 | −0.79 | −0.83 | −0.83 | −1.31 | −1.30 | −0.75 | −0.74 | −0.73 | −0.73 | −0.85 |
| Ca | −2.20 | −2.18 | −1.93 | −1.91 | −2.13 | −2.10 | −2.50 | −2.48 | −2.10 | −2.08 | −1.80 | −1.78 | −1.84 |
| Sr | −1.89 | −1.88 | −1.64 | −1.63 | −1.85 | −1.83 | −2.24 | −2.23 | −1.83 | −1.82 | −1.57 | −1.56 | −1.72 |
| Ba | −2.20 | −2.19 | −1.88 | −1.87 | −2.13 | −2.11 | −2.49 | −2.48 | −2.05 | −2.04 | −1.70 | −1.69 | −1.90 |
| Al | −4.00 | −3.96 | −3.47 | −3.44 | −3.85 | −3.81 | −4.25 | −4.20 | −3.66 | −3.62 | −3.43 | −3.39 | −3.39 |
| Pb | −3.78 | −3.77 | −3.02 | −3.01 | −3.40 | −3.39 | −3.59 | −3.58 | −3.01 | −3.00 | −2.93 | −2.93 | −2.03 |
| Fe | −6.40 | −6.35 | −4.94 | −4.90 | −5.67 | −5.63 | −5.03 | −4.99 | −4.57 | −4.53 | −3.31 | −3.27 | −4.28 |
| V | −6.74 | −6.71 | −5.42 | −5.39 | −6.02 | −5.99 | −6.21 | −6.17 | −4.58 | −4.54 | −3.61 | −3.58 | −5.31 |
| Mo | −8.09 | −8.05 | −6.34 | −6.30 | −7.15 | −7.11 | −6.98 | −6.95 | −5.66 | −5.63 | −5.25 | −5.22 | −6.82 |
| W | −10.23 | −10.19 | −8.46 | −8.43 | −9.26 | −9.23 | −9.95 | −9.92 | −8.73 | −8.70 | −7.81 | −7.78 | −8.90 |
| Nb | −8.50 | −8.47 | −7.04 | −7.01 | −7.76 | −7.73 | −7.91 | −7.88 | −6.56 | −6.53 | −6.21 | −6.18 | −7.57 |
| Ta | −9.59 | −9.56 | −8.19 | −8.17 | −9.01 | −8.99 | −8.76 | −8.74 | −8.46 | −8.44 | −7.77 | −7.75 | −8.09 |
| Ni | −6.09 | −6.05 | −4.76 | −4.72 | −5.49 | −5.45 | −4.95 | −4.91 | −4.53 | −4.49 | −3.26 | −3.22 | −4.44 |
| Cu | −4.54 | −4.51 | −3.52 | −3.49 | −4.03 | −3.99 | −4.28 | −4.25 | −3.94 | −3.90 | −3.10 | −3.07 | −3.49 |
| Rh | −7.58 | −7.55 | −5.83 | −5.80 | −6.72 | −6.68 | −5.60 | −5.57 | −5.29 | −5.26 | −4.82 | −4.79 | −5.75 |
| Ir | −9.32 | −9.29 | −7.45 | −7.42 | −8.48 | −8.45 | −7.16 | −7.13 | −7.55 | −7.52 | −6.41 | −6.38 | −6.94 |
| Pd | −5.06 | −5.02 | −3.72 | −3.70 | −4.46 | −4.43 | −4.08 | −4.05 | −4.31 | −4.28 | −2.98 | −2.96 | −3.89 |
| Pt | −7.15 | −7.12 | −5.59 | −5.56 | −6.50 | −6.48 | −5.81 | −5.79 | −5.86 | −5.84 | −5.47 | −5.45 | −5.84 |
| Ag | −3.63 | −3.60 | −2.54 | −2.52 | −3.11 | −3.09 | −3.17 | −3.15 | −2.89 | −2.87 | −2.44 | −2.42 | −2.95 |
| Au | −4.38 | −4.36 | −3.09 | −3.07 | −3.79 | −3.77 | −3.61 | −3.59 | −3.59 | −3.58 | −2.97 | −2.96 | −3.81 |
| Th | −7.54 | −7.53 | −6.37 | −6.35 | −7.25 | −7.23 | −6.83 | −6.82 | −6.44 | −6.43 | −6.06 | −6.05 | −6.20 |

TABLE VII. Equilibrium cohesive energies (eV/atom) of 40 non-metallic solids

| Solid | LDA | | PBE | | PBEsol | | M06-L | | SCAN | | HSE06 | | Exp.* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | Uncorr. | Corr. | |
| LiF | −4.92 | −4.86 | −4.36 | −4.30 | −4.51 | −4.45 | −4.53 | −4.47 | −4.38 | −4.32 | −4.27 | −4.21 | −4.40 |
| LiCl | −3.82 | −3.78 | −3.40 | −3.37 | −3.56 | −3.52 | −3.79 | −3.75 | −3.52 | −3.49 | −3.42 | −3.38 | −3.55 |
| NaF | −4.36 | −4.31 | −3.83 | −3.79 | −3.97 | −3.92 | −4.08 | −4.04 | −3.88 | −3.84 | −3.74 | −3.70 | −3.93 |
| NaCl | −3.48 | −3.45 | −3.11 | −3.09 | −3.24 | −3.21 | −3.59 | −3.57 | −3.28 | −3.25 | −3.13 | −3.11 | −3.33 |
| MgO | −5.80 | −5.72 | −4.98 | −4.91 | −5.31 | −5.24 | −5.25 | −5.18 | −5.19 | −5.11 | −4.91 | −4.84 | −5.12 |
| MgS | −4.31 | −4.27 | −3.71 | −3.67 | −4.03 | −3.99 | −4.10 | −4.05 | −3.97 | −3.93 | −3.76 | −3.71 | −4.00 |
| TiC | −8.63 | −8.55 | −7.43 | −7.35 | −8.01 | −7.92 | −7.79 | −7.71 | −7.08 | −7.00 | −7.30 | −7.21 | −7.16 |
| ZrC | −9.10 | −9.03 | −7.97 | −7.91 | −8.49 | −8.43 | −8.24 | −8.17 | −7.65 | −7.58 | −7.65 | −7.58 | −7.93 |
| HfC | −9.26 | −9.19 | −8.10 | −8.03 | −8.73 | −8.66 | −8.31 | −8.24 | −8.13 | −8.06 | −7.90 | −7.84 | −8.11 |
| VC | −8.34 | −8.27 | −7.07 | −7.01 | −7.68 | −7.61 | −7.31 | −7.24 | −6.62 | −6.55 | −6.12 | −6.05 | −6.94 |
| NbC | −9.34 | −9.27 | −7.99 | −7.92 | −8.65 | −8.58 | −8.27 | −8.20 | −7.69 | −7.62 | −7.53 | −7.46 | −8.26 |
| TiN | −8.29 | −8.21 | −7.02 | −6.95 | −7.58 | −7.51 | −7.25 | −7.18 | −6.60 | −6.53 | −6.76 | −6.68 | −6.69 |
| ZrN | −8.76 | −8.70 | −7.56 | −7.50 | −8.07 | −8.01 | −7.72 | −7.66 | −7.14 | −7.08 | −7.13 | −7.07 | −7.52 |
| HfN | −8.80 | −8.74 | −7.54 | −7.49 | −8.17 | −8.11 | −7.63 | −7.58 | −7.48 | −7.42 | −7.246 | −7.191 | −8.03 |
| VN | −7.63 | −7.57 | −6.31 | −6.26 | −6.90 | −6.84 | −6.38 | −6.33 | −5.77 | −5.72 | −5.20 | −5.14 | −6.25 |
| NbN | −8.52 | −8.49 | −7.11 | −7.08 | −7.76 | −7.72 | −7.25 | −7.22 | −6.71 | −6.68 | −6.51 | −6.48 | −7.50 |
| C | −8.94 | −8.76 | −7.73 | −7.55 | −8.28 | −8.10 | −7.48 | −7.30 | −7.54 | −7.36 | −7.57 | −7.39 | −7.37 |
| Si | −5.30 | −5.23 | −4.58 | −4.51 | −4.97 | −4.91 | −4.69 | −4.63 | −4.73 | −4.67 | −4.55 | −4.49 | −4.63 |
| Ge | −4.59 | −4.55 | −3.76 | −3.72 | −4.23 | −4.19 | −3.83 | −3.79 | −3.97 | −3.94 | −3.75 | −3.71 | −3.87 |
| Sn | −3.95 | −3.93 | −3.21 | −3.19 | −3.60 | −3.58 | −3.36 | −3.34 | −3.39 | −3.37 | −3.23 | −3.21 | −3.14 |
| AlP | −4.81 | −4.75 | −4.11 | −4.06 | −4.46 | −4.40 | −4.23 | −4.17 | −4.26 | −4.20 | −4.11 | −4.06 | −4.26 |
| AlAs | −4.46 | −4.42 | −3.71 | −3.67 | −4.08 | −4.03 | −3.83 | −3.78 | −3.87 | −3.83 | −3.74 | −3.70 | −3.78 |
| AlSb | −3.97 | −3.94 | −3.27 | −3.23 | −3.62 | −3.58 | −3.42 | −3.38 | −3.41 | −3.37 | −3.30 | −3.27 | −3.30 |
| BN | −8.05 | −7.89 | −7.01 | −6.85 | −7.41 | −7.25 | −6.76 | −6.61 | −6.83 | −6.68 | −6.79 | −6.64 | −6.60 |
| BP | −6.23 | −6.13 | −5.36 | −5.26 | −5.74 | −5.64 | −5.20 | −5.10 | −5.31 | −5.21 | −5.23 | −5.13 | −5.04 |
| AsB | −5.61 | −5.53 | −4.71 | −4.63 | −5.09 | −5.01 | −4.63 | −4.55 | −4.68 | −4.60 | −4.60 | −4.52 | −4.70 |
| GaN | −5.38 | −5.30 | −4.41 | −4.33 | −4.85 | −4.77 | −4.35 | −4.28 | −4.44 | −4.37 | −4.29 | −4.21 | −4.48 |
| GaP | −4.32 | −4.27 | −3.51 | −3.46 | −3.92 | −3.87 | −3.55 | −3.51 | −3.65 | −3.61 | −3.52 | −3.47 | −3.56 |
| GaAs | −4.04 | −4.00 | −3.17 | −3.14 | −3.58 | −3.55 | −3.26 | −3.23 | −3.32 | −3.29 | −3.21 | −3.17 | −3.31 |
| GaSb | −3.66 | −3.64 | −2.85 | −2.82 | −3.22 | −3.20 | −2.99 | −2.97 | −3.01 | −2.98 | −2.90 | −2.87 | −3.00 |
| InP | −3.96 | −3.92 | −3.17 | −3.14 | −3.56 | −3.52 | −3.27 | −3.23 | −3.27 | −3.23 | −3.19 | −3.15 | −3.43 |
| InAs | −3.74 | −3.71 | −2.92 | −2.89 | −3.30 | −3.28 | −3.04 | −3.01 | −3.02 | −2.99 | −2.94 | −2.91 | −3.05 |
| InSb | −3.45 | −3.43 | −2.67 | −2.65 | −3.04 | −3.02 | −2.86 | −2.84 | −2.79 | −2.77 | −2.73 | −2.71 | −2.79 |
| SiC | −7.40 | −7.28 | −6.41 | −6.30 | −6.88 | −6.77 | −6.45 | −6.34 | −6.47 | −6.36 | −6.35 | −6.24 | −6.36 |
| ZnS | −3.71 | −3.67 | −2.91 | −2.87 | −3.30 | −3.26 | −3.06 | −3.02 | −3.15 | −3.11 | −2.96 | −2.93 | −3.17 |
| ZnSe | −3.37 | −3.34 | −2.58 | −2.55 | −2.98 | −2.95 | −2.63 | −2.60 | −2.80 | −2.77 | −2.66 | −2.63 | −2.63 |
| ZnTe | −2.95 | −2.93 | −2.11 | −2.09 | −2.26 | −2.24 | −2.19 | −2.17 | −2.31 | −2.29 | −1.99 | −1.97 | −2.41 |
| CdS | −3.32 | −3.28 | −2.57 | −2.53 | −2.92 | −2.89 | −2.77 | −2.74 | −2.76 | −2.72 | −2.64 | −2.61 | −2.78 |
| CdSe | −3.07 | −3.04 | −2.32 | −2.30 | −2.68 | −2.66 | −2.43 | −2.41 | −2.49 | −2.47 | −2.41 | −2.39 | −2.46 |
| CdTe | −2.74 | −2.72 | −1.93 | −1.91 | −2.05 | −2.03 | −2.08 | −2.06 | −2.09 | −2.07 | −1.87 | −1.85 | −2.23 |

* LiF[83], LiCl[83], NaF[83], NaCl[83], MgO[62], MgS[84,85], TiC[83,86], ZrC[83,86,87], HfC[83,86], VC[83,86], NbC[83,86,87], TiN[88], ZrN[87], HfN[89], VN[88], NbN[87], C[82], Si[82], Ge[82], Sn[82], SiC[83,90], AlP[91], AlAs[91], AlSb[92], BN[83,90], BP[92], BAs(300 K)[93], GaN[83,90], GaP[83,90], GaAs[77], GaSb[94], InP[94], InAs[94], InSb[94], ZnS[92,95], ZnSe[92,95], ZnTe[92,95], CdS[92], CdSe[92], CdTe[92].

TABLE VIII. The mean absolute relative error (MARE, %) for the lattice constants $a_0$, cohesive energies $E_0$, and bulk moduli $B_0$ of the 23 semiconductor solids.

| | LDA | PBE | PBEsol | M06-L | SCAN | HSE06 |
|---|---|---|---|---|---|---|
| $a_0$ | 0.6 | 1.5 | 0.4 | 1.6 | 0.5 | 0.8 |
| $E_0$ | 19.1 | 5.2 | 7.4 | 2.5 | 2.2 | 4.7 |
| $B_0$ | 4.1 | 15.3 | 5.5 | 12.2 | 3.6 | 5.3 |
| | | PBE+vdW | | M06-L+vdW | | HSE06+vdW |
| $a_0$ | | 0.7 | | 1.0 | | 0.3 |
| $E_0$ | | 3.6 | | 5.2 | | 4.1 |
| $B_0$ | | 7.8 | | 9.4 | | 4.3 |

TABLE IX. $k$-point meshes (kpts) settings for FHI-aims tier 2 calculations within LDA, GGAs, and MGGAs. For the hybrid HSE06 calculations, coarser densities are used due to the excessive computational cost.

| Solid | kpts | Solid | kpts |
|---|---|---|---|
| Li | 32×32×32 | HfC | 22×22×22 |
| Na | 28×28×28 | VC | 24×24×24 |
| K | 22×22×22 | NbC | 22×22×22 |
| Rb | 22×22×22 | TiN | 24×24×24 |
| Ca | 18×18×18 | ZrN | 22×22×22 |
| Sr | 18×18×18 | HfN | 22×22×22 |
| Ba | 24×24×24 | VN | 24×24×24 |
| Al | 24×24×24 | NbN | 22×22×22 |
| Pb | 20×20×20 | C | 46×46×46 |
| Fe | 38×38×38 | Si | 28×28×28 |
| V | 36×36×36 | Ge | 32×32×32 |
| Mo | 36×36×36 | Sn | 26×26×26 |
| W | 36×36×36 | AlP | 16×16×16 |
| Nb | 34×34×34 | AlAs | 16×16×16 |
| Ta | 34×34×34 | AlSb | 14×14×14 |
| Ni | 28×28×28 | BN | 24×24×24 |
| Cu | 28×28×28 | BP | 20×20×20 |
| Rh | 26×26×26 | BAs | 20×20×20 |
| Ir | 26×26×26 | GaN | 20×20×20 |
| Pd | 26×26×26 | GaP | 16×16×16 |
| Pt | 26×26×26 | GaAs | 16×16×16 |
| Ag | 24×24×24 | GaSb | 16×16×16 |
| Au | 24×24×24 | InP | 16×16×16 |
| Th | 20×20×20 | InAs | 16×16×16 |
| LiF | 24×24×24 | InSb | 14×14×14 |
| LiCl | 20×20×20 | SiC | 20×20×20 |
| NaF | 22×22×22 | ZnS | 16×16×16 |
| NaCl | 18×18×18 | ZnSe | 16×16×16 |
| MgO | 24×24×24 | ZnTe | 16×16×16 |
| MgS | 20×20×20 | CdS | 16×16×16 |
| TiC | 24×24×24 | CdSe | 16×16×16 |
| ZrC | 22×22×22 | CdTe | 14×14×14 |

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