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# Accurate values of 3C, 2H, 4H, and 6H SiC elastic constants using DFT calculations and heuristic errors corrections

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**ABSTRACT**

Silicon carbide is an important material with applications in numerous domains, but for which our knowledge of basic properties like elastic constants is surprisingly limited. Although several density functional theory calculations have been reported, those are usually not accurate enough, with a sizeable dispersion of published values. A heuristic method is proposed here, allowing for largely reducing the uncertainty. It is based on the use of a weighted average of errors for two reference materials, Si and C. It is demonstrated that this method is effective for physical properties like the lattice parameter and the bulk modulus. It is then used for determining the full sets of elastic constants for the 3C, 2H, 4H, and 6H silicon carbide polytypes.

Silicon carbide, a ceramic compound, has found its way in various applications, in particular as an abrasive and a structural material due to its excellent mechanical properties [1]. It is also used in high-frequency or high temperature electronic devices. Its high resistance to radiation makes it a potential key component in nuclear applications [2]. Finally, SiC is bio-compatible and interesting for biosensor applications [3]. It is then not surprising to find an abundance of dedicated studies in the literature.

It is however surprising that despite of all these works, basic SiC properties like the elastic constants are still not known with a high accuracy. Table 1 shows available data, both from experiments and calculations, for the most common polytypes. It appears clearly that measured values are scarce, and are associated to a non negligible uncertainty. There are also no reported values for 2H SiC. One of the main issue for these measurements is the lack of monocrystalline samples with very high crystalline quality and of large enough dimensions. Numerical simulations offer an alternative to this issue, but the ranges of reported values are often large, even when obtained using first principles

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**Table 1.** Elastic constants values reported in the literature for 3C, 2H, 4H and 6H SiC.

| | Ref. | $C_{11}$ | $C_{12}$ | $C_{13}$ | $C_{33}$ | $C_{44}$ |
|---|---|---|---|---|---|---|
| 3C | Exp. [4] | 395 ± 12 | 132 ± 9 | | | 236 ± 7 |
| | Exp. [5] | 390 | 142 | | | 256 |
| | The. [1, 5–12] | 300–451 (352–420) | 101–214 (126–163) | | | 136–287 (211–287) |
| 2H | The. [1, 11–13] | 388–541 (499–541) | 93–183 (93–117) | 49–139 (49–61) | 422–586 (533–586) | 127–162 (156–162) |
| 4H | Exp. [14] | 507 ± 6 | 108 ± 8 | 52 ± 9 | 547 ± 6 | 159 ± 7 |
| | Exp. [15] | | | | 605.2 ± 1 | |
| | The. [1, 9, 12] | 495–534 (498–534) | 91–187 (91–96) | 50–159 (50–52) | 535–577 (535–574) | 142–171 (171) |
| 6H | Exp. [14] | 501 ± 4 | 111 ± 5 | 52 ± 9 | 553 ± 4 | 163 ± 4 |
| | Exp. [16] | 502 ± 20 | 95 ± 29 | | 565 ± 11 | 169 ± 4 |
| | Exp. [15] | | | | 551.2 ± 8.3 | |
| | The. [1, 8] | 498–527 (527) | 107–186 (107) | 56–176 (56) | 563–567 (563) | 141–165 (165) |

Notes: The experimental uncertainty is indicated when provided by the authors. For theoretical values, the range of all reported values is given (in parenthesis the range of values obtained using first-principles calculations).

calculations. For instance, reported ranges for 3C $C_{11}$ and $C_{44}$ values are greater than 60 GPa. It would then be highly desirable to determine more accurate values of these elastic constants.

Unfortunately, there are not many practical solutions. The determination of elastic constants requires an accurate calculation of the second-order derivative of the energy relatively to the strain. For density functional theory (DFT), this quantity considerably depends on the functional used to describe exchange correlation (XC) contributions. This partially explains the dispersion of values reported in the literature. Other first principle methods like quantum Monte Carlo or other wavefunction based quantum chemistry approaches are more accurate than DFT. However they are not well suited for periodic system calculations and for computing elastic constants.

In this work we describe a heuristic method allowing for correcting DFT computed elastic constants in silicon carbide. It is based on estimating the error associated to the XC functional from a weighted average of the errors computed for Si and C as references. The gain in accuracy is demonstrated in the case of the lattice parameter and the bulk modulus, using data from the literature. Then the method is applied to determine the elastic constants of 3C, 2H, 4H and 6H SiC, by correcting DFT calculations carried out with six different XC functionals.

First, let $X_{AB}$ be the value of a given property for an AB alloy, such as the lattice parameter or the bulk modulus. Let us assume that $X_{AB}$ can be expressed as the weighted average of the same quantity for its constituent materials A and B. For cubic SiC, for instance, one can write

$$X_{SiC} = \alpha X_C + (1 - \alpha)X_{Si} \tag{1}$$

Knowing $X_{SiC}$, $X_{Si}$ and $X_C$ values, $\alpha$ is obtained with

$$\alpha = \frac{X_{SiC} - X_{Si}}{X_C - X_{Si}} \tag{2}$$

For instance, $\alpha = 0.575$ for the lattice parameter and $\alpha = 0.362$ for the bulk modulus. Next, let $\widetilde{X}$ be the DFT computed value of the property $X$. The error compared to the correct reference value is

$$\Delta = \widetilde{X} - X \tag{3}$$

$\Delta$ depends on the considered property as well as on material. It also critically depends on the exchange correlation functional used in the DFT calculation. Now, for the property $X$ and a given exchange correlation functional, let us assume that $\Delta$ for 3C-SiC can be computed using a weighted average

$$\Delta_{SiC} = \alpha \Delta_C + (1 - \alpha)\Delta_{Si} \tag{4}$$

with $\alpha$ obtained from Equation (2). Knowing $\Delta_{SiC}$ would then allow for

determining an error-corrected value $X^*_{\mathrm{SiC}}$ from

$$X^*_{\mathrm{SiC}} = \widetilde{X}_{\mathrm{SiC}} - \Delta_{\mathrm{SiC}} \qquad (5)$$

This assumption is tested for three properties, the lattice parameter, the cohesive energy and the bulk modulus, and different exchange correlation functionals. Figure 1 compares both original DFT ($\widetilde{X}$) and corrected values ($X^*$) using data compiled by Tran et al. [17]. For each property, $\alpha$ is computed with Equation (2) and reference values for C, Si, and 3C-SiC (given in Ref. [17]). For each functional, the corrected value is obtained from Equation (5), $\Delta_{\mathrm{SiC}}$ being calculated using Equation (4). Figure 1 clearly shows that a significant improvement is achieved for most functionals for the three quantities. Going deeper into the analysis, it appears that for the lattice parameter and the bulk modulus, an impressive agreement is obtained for LDA, GGA functionals, and their hybrid versions (left part of the graphs). It is less satisfactory for dispersion-corrected functionals (right part). A quantitative assessment of the correction is obtained by calculating the mean average errors (MAE) for the different sets of data (Table 2). The MAE are significantly reduced for all datasets, which confirms the visual impression in Figure 1.

This analysis confirms that our assumption is correct for the considered properties, and that Equations (4) and (5) can be used to correct DFT data for SiC. In other words, it is shown that the DFT errors for SiC can be approximated by a weighted average of the DFT errors for Si and C, at least for quantities like lattice parameter, cohesive energy, and bulk modulus.

Note that for computing the weight factor $\alpha$, one needs to know the value of the desired SiC quantity (Equation (2)). However, it can be shown that a
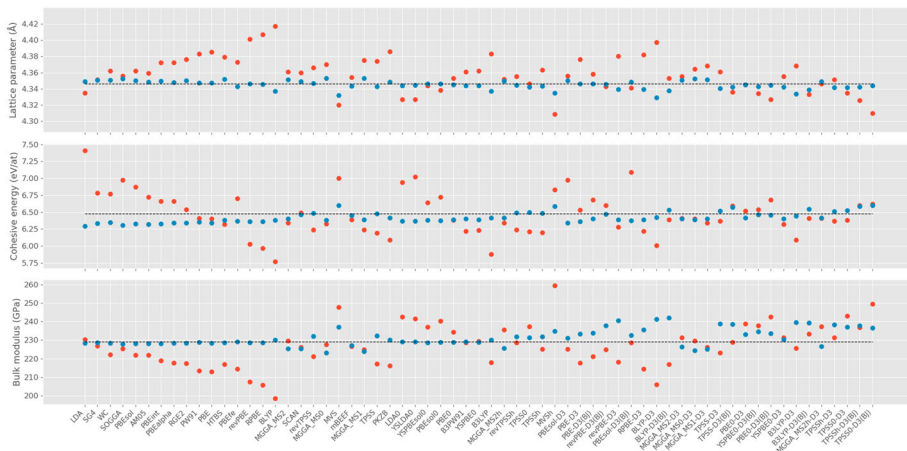


**Figure 1.** DFT calculated values for SiC lattice parameter (top), cohesive energy (middle), and bulk modulus (bottom), for various exchange correlation functionals (data from Ref. [17]). Red dots correspond to the original data, and blue dots to corrected values using Equation (5). The dashed lines show the experimental reference values.

**Table 2.** Mean average errors (MAE) for 3C-SiC lattice parameter $a_0$, cohesive energy $E_{coh}$ and bulk modulus B from original data reported in Ref. [18] (4 XC functionals), Ref. [17] (63 XC functionals), and Ref. [19] (18 XC functionals), as well as MAE for corrected values (see text for details).

|  |  | $a_0$ (Å) | $E_{coh}$ (eV) | B (GPa) |
|---|---|---|---|---|
| Ref. [18] | Orig. | 0.0118 | 0.157 | 7.520 |
|  | Corr. | 0.0019 | 0.091 | 1.208 |
| Ref. [17] | Orig. | 0.0200 | 0.245 | 8.859 |
|  | Corr. | 0.0041 | 0.085 | 3.669 |
| Ref. [17]* | Orig. | 0.0240 | 0.315 | 10.348 |
|  | Corr. | 0.0029 | 0.118 | 0.556 |
| Ref. [19] | Orig. | 0.0258 | 0.237 | 11.042 |
|  | Corr. | 0.0027 | 0.090 | 1.931 |

Note: The values corresponding to a subset of 24 XC functionals from Ref. [17] are also reported.

relevant error reduction can be achieved even with an approximate value. Figure 2 represents the variation of the MAE using a weight factor $\alpha$ ranging from 0 to 1, and using data from Ref. [17] (a similar picture is obtained for all datasets). Two findings stand out. First, for the lattice parameter and the bulk modulus, the lowest MAE are obtained for $\alpha$ computed using Equation
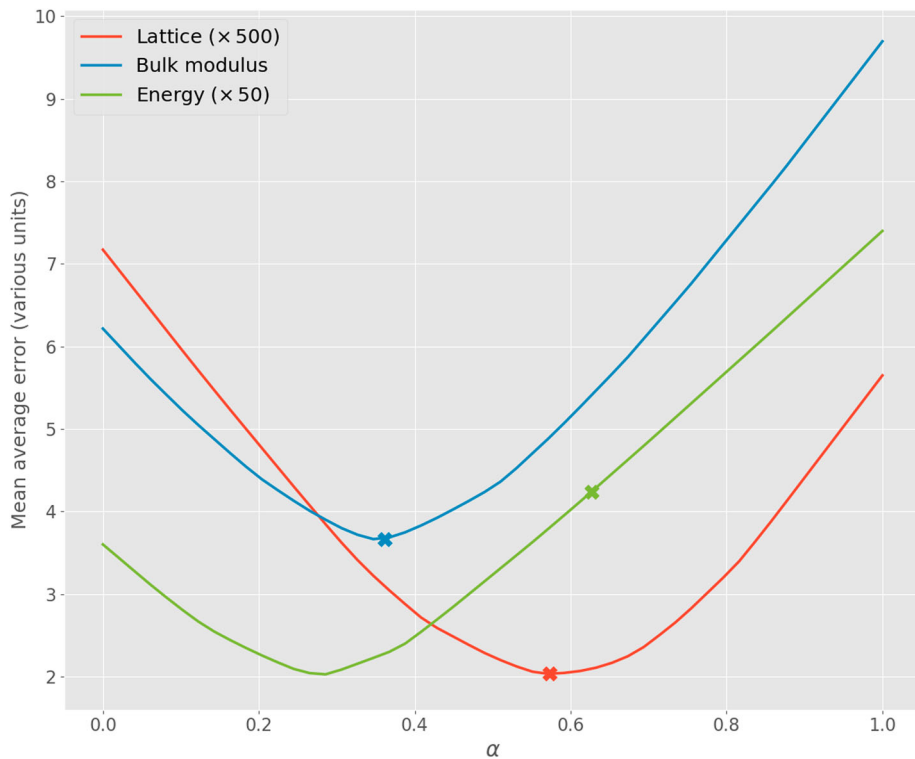


**Figure 2.** Variations of mean average error (MAE) for three 3C-SiC quantities, with corrections using a weight factor $a$ ranging from 0 to 1 and Equation 4, using data reported in Ref. [17]. The crosses show the MAE with corrections using $a$ computed using Equation (2). Values for lattice parameter (cohesive energy) were multiplied by 500 (50) for the sake of comparison.

(2). This is not true for cohesive energy. This is probably related to the fact that there is an energy gain by forming SiC from its constituents, which is not described by Equation (1). Second, for lattice parameter and bulk modulus, it appears that significant errors corrections can be obtained even when $\alpha$ is close but not equal to the ideal value given by Equation (2). Therefore the error correction scheme proposed in this work can be employed even if only approximate $X_{SiC}$ data are available.

The DFT calculations were performed using the Quantum Espresso package [22]. Overestimated parameters were used whenever possible in order to minimize computational errors. For instance, excellent convergence was obtained with plane-wave and charge density cutoffs of 90 and 720 Ry. The Brillouin zone sampling was achieved with k-points grids of $12 \times 12 \times 12$ for 3C (2 atoms) and 2H (4 atoms), $12 \times 12 \times 6$ for 4H (8 atoms), and $12 \times 12 \times 4$ for 6H (12 atoms). An initial variable cell optimization was performed to determine the lattice parameters, with convergence thresholds of $10^{-9}$ eV for the energy, $3 \times 10^{-5}$ eV Å$^{-1}$ for forces, and $10^{-4}$ GPa for cell stress components. The second-order elastic constants were next determined using the ElaStic tool [23], with DFT convergence thresholds of $10^{-9}$ eV for the energy and $3 \times 10^{-3}$ eV Å$^{-1}$ for forces. The range of applied strains was $\pm 0.06$, and elastic constants were computed by fitting the energies of the strained cells using $6^{th}$-order polynomials. We checked that these parameters were appropriate to obtain extremely well converged elastic constants (Tables 3 and 4).

Regarding the choice of the exchange correlation (XC) functionals, it is important to emphasize that we aim at determining accurate values for SiC polytypes elastic constants, and not at assessing the accuracy of a large set of these functionals. However, several ones should be considered to gain confidence in the robustness of our results. As a compromise, six different XC functionals (LDA [24, 25], PBE [26], PBEsol [27], revPBE [28], optB88 [29], and optB86bb [30]) were selected. In particular, we found that bulk modulus values computed with these functionals match closely the reference data, with differences lower than 1 GPa, when the corrections described in the previous section are applied.

**Table 3.** Lattice parameter and elastic constants (raw and corrected values) for 3C-SiC from DFT calculations with different XC functionals.

| 3C-SiC | $a_0$ (Å) | $C_{11}$ (GPa) | | $C_{12}$ (GPa) | | $C_{44}$ (GPa) | |
|---|---|---|---|---|---|---|---|
| | | Raw | Corr. | Raw | Corr. | Raw | Corr. |
| LDA | 4.3288 | 403.8 | 403.1 | 142.3 | 112.3 | 253.7 | 253.2 |
| PBE | 4.3805 | 383.9 | 401.8 | 127.6 | 124.7 | 239.5 | 251.3 |
| PBEsol | 4.3575 | 390.9 | 401.3 | 138.0 | 116.7 | 243.4 | 249.7 |
| optB88 | 4.3721 | 387.5 | 402.9 | 129.5 | 122.0 | 241.9 | 251.7 |
| optB86b | 4.3663 | 385.8 | 400.3 | 135.6 | 117.2 | 240.3 | 248.8 |
| revPBE | 4.3966 | 377.2 | 401.5 | 122.7 | 128.5 | 235.3 | 250.6 |
| Avg. | | 388.2 | **400.3** | 132.6 | **120.2** | 242.3 | **250.9** |
| Std. Dev. | | 8.1 | 1.0 | 6.6 | 5.4 | 5.7 | 1.4 |

**Table 4.** DFT calculated lattice parameters and elastic constants for C and Si with different XC functionals, and experimental reference values for C [20] and Si [21] elastic constants.

| | C | | | | Si | | | |
|---|---|---|---|---|---|---|---|---|
| | $a_0$ (Å) | $C_{11}$ (GPa) | $C_{12}$ (GPa) | $C_{44}$ (GPa) | $a_0$ (Å) | $C_{11}$ (GPa) | $C_{12}$ (GPa) | $C_{44}$ (GPa) |
| Ref. | | 1080.9 | 125.0 | 578.9 | | 167.54 | 64.92 | 80.24 |
| LDA | 4.3288 | 1102.4 | 148.3 | 591.0 | 5.3995 | 161.6 | 64.4 | 74.4 |
| PBE | 4.3805 | 1051.7 | 125.5 | 557.6 | 5.4692 | 153.3 | 56.8 | 73.6 |
| PBEsol | 4.3575 | 1071.0 | 141.1 | 573.3 | 5.4325 | 157.0 | 62.6 | 73.6 |
| optB88 | 4.3721 | 1057.7 | 129.3 | 561.4 | 5.4571 | 154.6 | 58.0 | 74.6 |
| optB86b | 4.3663 | 1059.5 | 138.5 | 567.8 | 5.4440 | 155.3 | 61.2 | 73.1 |
| revPBE | 4.3966 | 1033.6 | 118.1 | 547.0 | 5.4919 | 150.6 | 54.0 | 73.9 |

The full-potential projector augmented wave method was used to compute the electron-ion interactions [31]. Pseudopotentials for C and Si, generated for LDA, PBE, and PBEsol functionals, were selected from the PSlibrary [32]. For the calculations with the revPBE, optB88 and optB86B functionals, the PBE pseudopotential was used. Note that all calculations were carried out with the scalar relativistic version of these pseudopotentials, since tests made with full relativistic pseudopotentials resulted in negligible differences.

There is an additional hurdle for computing the elastic constants of the hexagonal polytypes. In fact, accurate reference values of the elastic constants of hexagonal diamond and silicon are not available. A way to circumvent this issue is to transform the cubic elastic constants for Si and C into their hexagonal counterparts, using the known relations [33] reported below:

$$C_{11}^{H} = \frac{1}{6}(3C_{11} + 3C_{12} + 6C_{44}) \tag{6}$$

$$C_{12}^{H} = \frac{1}{6}(C_{11} + 5C_{12} - 2C_{44}) \tag{7}$$

$$C_{13}^{H} = \frac{1}{6}(2C_{11} + 4C_{12} - 4C_{44}) \tag{8}$$

$$C_{33}^{H} = \frac{1}{6}(2C_{11} + 4C_{12} + 8C_{44}) \tag{9}$$

$$C_{44}^{H} = \frac{1}{6}(2C_{11} - 2C_{12} + 2C_{44}) \tag{10}$$

Such a transformation is accurate if internal strains in the hexagonal phase are negligible, which we assume to be the case for elemental materials like C and Si. The raw and corrected DFT results for 2H, 4H and 6H SiC are reported in Tables 5, 6, and 7. A large reduction of the standard deviation is clearly obtained for $C_{11}$ and $C_{33}$, and to a lesser extent for $C_{13}$ and $C_{44}$. Only for $C_{12}$ the improvement is moderate, as for 3C-SiC. Our values are in excellent agreement with experiments by Kamitani et al. [14], except for $C_{12}$. It is not clear if the discrepancy is related to the correction scheme or to the experiments. Arlt

**Table 5.** Lattice parameters and elastic constants (raw and corrected values) for 2H-SiC from DFT calculations with different XC functionals.

| 2H-SiC | $a_0$ (Å) | $c_0/a_0$ | $C_{11}$ (GPa) | | $C_{12}$ (GPa) | | $C_{13}$ (GPa) | | $C_{33}$ (GPa) | | $C_{44}$ (GPa) | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Raw | Corr. | Raw | Corr. | Raw | Corr. | Raw | Corr. | Raw | Corr. |
| LDA | 3.0562 | 1.64123 | 522.9 | 518.5 | 114.4 | 85.4 | 58.1 | 49.7 | 566.7 | 560.0 | 155.7 | 157.8 |
| PBE | 3.0905 | 1.64124 | 495.9 | 519.2 | 102.7 | 94.9 | 51.3 | 51.5 | 535.2 | 560.7 | 151.7 | 158.8 |
| PBEsol | 3.0763 | 1.64113 | 504.1 | 513.9 | 111.1 | 89.3 | 57.8 | 52.2 | 545.6 | 554.7 | 150.1 | 156.3 |
| optB88 | 3.0864 | 1.64144 | 498.4 | 517.5 | 103.4 | 91.6 | 51.3 | 50.2 | 538.3 | 558.8 | 152.2 | 158.6 |
| optB86b | 3.0826 | 1.64101 | 497.7 | 512.8 | 109.1 | 90.1 | 56.7 | 52.7 | 538.3 | 553.3 | 148.5 | 156.0 |
| revPBE | 3.1038 | 1.64113 | 483.8 | 516.0 | 97.4 | 96.7 | 47.9 | 51.6 | 521.3 | 556.9 | 149.7 | 158.3 |
| Avg. | 3.0826 | | 500.5 | **516.3** | 106.3 | **91.3** | 53.8 | **51.3** | 540.9 | **557.4** | 151.3 | **157.7** |
| Std. Dev. | | | 11.7 | 2.3 | 5.7 | 3.7 | 3.9 | 1.1 | 13.6 | 2.7 | 2.3 | 1.1 |

**Table 6.** Lattice parameters and elastic constants (raw and corrected values) for 4H-SiC from DFT calculations with different XC functionals.

| 4H-SiC | $a_0$ (Å) | $c_0/a_0$ | $C_{11}$ (GPa) | | $C_{12}$ (GPa) | | $C_{13}$ (GPa) | | $C_{33}$ (GPa) | | $C_{44}$ (GPa) | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Raw | Corr. | Raw | Corr. | Raw | Corr. | Raw | Corr. | Raw | Corr. |
| LDA | 3.0583 | 3.27373 | 515.9 | 511.5 | 118.5 | 89.5 | 59.2 | 50.8 | 566.3 | 559.6 | 163.1 | 165.2 |
| PBE | 3.0946 | 3.27389 | 486.7 | 510.0 | 104.5 | 96.7 | 51.7 | 51.9 | 532.0 | 557.5 | 157.6 | 164.7 |
| PBEsol | 3.0784 | 3.27364 | 497.6 | 507.4 | 114.4 | 92.6 | 58.7 | 53.1 | 545.8 | 554.9 | 157.1 | 163.3 |
| optB88 | 3.0886 | 3.27404 | 491.8 | 510.9 | 106.4 | 94.6 | 52.6 | 51.5 | 538.0 | 558.5 | 158.8 | 165.2 |
| optB86b | 3.0847 | 3.27351 | 491.2 | 506.3 | 112.4 | 93.3 | 57.6 | 53.6 | 538.6 | 553.6 | 155.3 | 162.8 |
| revPBE | 3.1059 | 3.27377 | 477.4 | 509.6 | 100.2 | 99.5 | 49.1 | 52.8 | 521.2 | 556.9 | 155.9 | 164.5 |
| Avg. | | | 493.4 | **509.3** | 109.4 | **94.4** | 54.8 | **52.3** | 540.3 | **556.8** | 158.0 | **164.3** |
| Std. Dev. | | | 11.8 | 1.8 | 6.2 | 3.1 | 3.9 | 1.0 | 13.8 | 2.0 | 2.6 | 0.9 |

**Table 7.** Lattice parameters and elastic constants (raw and corrected values) for 6H-SiC from DFT calculations with different XC functionals.

| 6H-SiC | $a_0$ (Å) | $c_0/a_0$ | $C_{11}$ (GPa) | | $C_{12}$ (GPa) | | $C_{13}$ (GPa) | | $C_{33}$ (GPa) | | $C_{44}$ (GPa) | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Raw | Corr. | Raw | Corr. | Raw | Corr. | Raw | Corr. | Raw | Corr. |
| LDA | 3.0591 | 4.90676 | 512.9 | 508.5 | 119.5 | 90.5 | 59.6 | 51.2 | 566.8 | 560.1 | 165.8 | 167.9 |
| PBE | 3.0955 | 4.90688 | 483.9 | 507.2 | 105.4 | 97.6 | 52.1 | 52.3 | 532.1 | 557.6 | 159.9 | 167.0 |
| PBEsol | 3.0793 | 4.90666 | 494.9 | 504.7 | 115.4 | 93.6 | 59.0 | 53.4 | 546.3 | 555.4 | 159.6 | 165.8 |
| optB88 | 3.0895 | 4.90708 | 489.1 | 508.2 | 107.2 | 95.4 | 53.1 | 52.0 | 538.3 | 558.8 | 161.2 | 167.6 |
| optB86b | 3.0855 | 4.90654 | 488.6 | 503.7 | 113.4 | 94.4 | 57.9 | 53.9 | 539.1 | 554.1 | 157.8 | 165.3 |
| revPBE | 3.1069 | 4.90680 | 474.9 | 507.1 | 101.0 | 100.3 | 49.6 | 53.3 | 521.5 | 557.2 | 158.2 | 166.8 |
| Avg. | | | 490.7 | **506.6** | 110.3 | **95.3** | 55.2 | **52.7** | 540.7 | **557.2** | 160.4 | **166.8** |
| Std. Dev. | | | 11.6 | 1.8 | 6.3 | 3.1 | 3.8 | 0.9 | 13.9 | 2.0 | 2.7 | 0.9 |

and Schodder reported a $C_{12}$ value close to ours, but associated to a significant error [16]. Finally, a value of 203.5 GPa for $C_{66}$ was recently reported [34] for 4H SiC. Since $C_{66} = (C_{11} - C_{12})/2$, it would suggest that $C_{12} = 102$ GPa using our $C_{11}$ value, or $C_{12} = 100$ GPa if $C_{11} = 507$ GPa as in Ref. [14]. Finally, Karmann et al. measured $C_{33} = 551.2$ GPa and $C_{33} = 605.2$ GPa in 6H and 4H, respectively Table 1. While their 6H value is comparable to ours and to previous works, the second one is probably overestimated.

Since we have now a full set of accurate elastic constants for several polytypes, it is interesting to examine trends. We note that there is a slight decrease for $C_{11}$ from 2H to 6H. Conversely, shear-related constants like $C_{12}$ and $C_{44}$ increase. No obvious variation exist for $C_{13}$ and $C_{33}$. Overall, the differences between hexagonal polytypes remain small.

In this work, we have presented a heuristic method allowing for computing elastic constants in different SiC polytypes with an unprecedented accuracy. This method is based on a determination of the error associated to density functional theory calculations from a weighted average of equivalent errors estimated for Si and C, two materials for which accurate data are available. The validity of the approach is demonstrated for the lattice parameter and the bulk modulus. In the case of elastic constants, it is shown that a significant reduction of the dispersion of DFT computed values is obtained in all cases, except for the $C_{12}$ constant for which the improvement is marginal. As a result, the full sets of elastic constants for 3C, 2H, 4H, and 6H were determined. Our results are in excellent agreement with experimental values from Kamitani et al. for 6H and 4H polytypes [14], and fill a gap for 2H and 3C for which there are few or no available data.

## Disclosure statement

No potential conflict of interest was reported by the author(s).

## Data availability statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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