Supporting Information

Insight into the inclusion of heteroatom impurities in Silicon structures

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Contents

1 Reference systems ................................. 2
1.1 Bulk systems ........................................ 2
1.2 Molecular systems .................................. 2
1.3 Silicon grain boundary without/with defects ...... 2

2 Systems with interstitial carbon impurities ......... 3
2.1 Electronic properties ................................. 3
2.2 Bonding analysis .................................... 4

3 Systems with interstitial nitrogen impurities ...... 9
3.1 Electronic properties ................................. 9
3.2 Bonding analysis .................................... 9

4 Systems with interstitial oxygen impurities ...... 14
4.1 Electronic properties ................................. 14
4.2 Bonding analysis .................................... 14

5 Bond charge variations ............................... 19
5.1 Nitrogen ............................................. 19
5.2 Oxygen ............................................... 23

6 Bond length variations ............................... 27
6.1 Carbon ............................................... 27
6.2 Nitrogen ............................................... 29
6.3 Oxygen ............................................... 34
1 Reference systems

1.1 Bulk systems

![Figure 1: Bonds and lone pairs on (a) SiC (b) SiO\textsubscript{2} (c) Si\textsubscript{3}N\textsubscript{4} (d) Diamond](image)

|                  | Si  | SiC | SiO\textsubscript{2} | Si\textsubscript{3}N\textsubscript{4} | Diamond |
|------------------|-----|-----|----------------------|---------------------------------------|----------|
| Bond Charges(BC) | 1.999 | 2.000 | 1.908, 1.957 | 2.313 | 1.999 |
| Bond length(BL)Å | 2.351 | 1.896 | 1.625, 1.628 | 1.747 | 1.547 |
| Lone Pair(LP)    |     |     | 4.1340 | N\textsubscript{2}:(0.5289 each) | 1.0578   |

Table 1: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-C, Si-O, Si-N and C-C bond from respective bulk systems: Si, SiC, SiO\textsubscript{2}, Si\textsubscript{3}N\textsubscript{4} and diamond.

1.2 Molecular systems

|                  | Ethane | Ethylene | Cyclopropane | Cyclopropene | Bicyclobutane |
|------------------|--------|----------|--------------|--------------|---------------|
| Bond Charges(BC) | 1.81   | 3.42     | 1.70         | 1.80, 3.20   | 1.87, 1.72    |
| Bond length(BL)Å | 1.53   | 1.33     | 1.52         | 1.53, 1.30   | 1.46, 1.55    |

Table 2: Bond charge(BC), bond length (BL) of molecular systems

1.3 Silicon grain boundary without/with defects
Table 3: Bond charge (BC), bond length (BL) and lone pair (LP) data for Si-Si bond without/with vacancy defect on Si-GB.

|                | Bond Charges (BC) | Bond length (BL) Å | LP  |
|----------------|-------------------|--------------------|-----|
| Si-GB: V1      | 2.00329           | 2.35084            |     |
|                | 2.00096           | 2.35122            |     |
|                | 1.98795           | 2.36642            |     |
| Si-GB: V2      | 2.0697            | 2.32564            | Si1: 0.99 |
|                | 2.0138            | 2.37601            | Si2: 1.00 |
|                | 2.0138            | 2.37601            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0712            | 2.31773            |     |
|                | 2.0712            | 2.31773            |     |
|                | 1.9712            | 2.42741            |     |
|                | 2.0282            | 2.47125            |     |
|                | 2.0062            | 2.50193            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0712            | 2.31773            |     |
|                | 2.0712            | 2.31773            |     |
|                | 1.9712            | 2.42741            |     |
|                | 2.0282            | 2.47125            |     |
|                | 2.0062            | 2.50193            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0712            | 2.31773            |     |
|                | 2.0712            | 2.31773            |     |
|                | 1.9712            | 2.42741            |     |
|                | 2.0282            | 2.47125            |     |
|                | 2.0062            | 2.50193            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0712            | 2.31773            |     |
|                | 2.0712            | 2.31773            |     |
|                | 1.9712            | 2.42741            |     |
|                | 2.0282            | 2.47125            |     |
|                | 2.0062            | 2.50193            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0712            | 2.31773            |     |
|                | 2.0712            | 2.31773            |     |
|                | 1.9712            | 2.42741            |     |
|                | 2.0282            | 2.47125            |     |
|                | 2.0062            | 2.50193            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0192            | 2.36607            |     |
|                | 2.0712            | 2.31773            |     |
|                | 2.0712            | 2.31773            |     |
|                | 1.9712            | 2.42741            |     |
|                | 2.0282            | 2.47125            |     |
|                | 2.0062            | 2.50193            |     |
|                | 2.0280            | 2.31424            |     |
|                | 2.0280            | 2.31424            |     |

Table 4: Formation energy (eV) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial C atoms from 1 to 4. The values are reported for the lowest energy structures.

| X  | $E_{i}^{XB}$ | $E_{i}^{XGB}$ | $E_{i}^{XV1GB}$ | $E_{i}^{XV2GB}$ |
|----|--------------|---------------|-----------------|-----------------|
| 1C | 3.5467       | 3.5072        | -1.6935         | -1.8003         |
| 2C | 4.6315       | 4.3359        | 0.4985          | 0.2165          |
| 3C | 6.2242       | 5.2122        | 0.9758          | 0.8144          |
| 4C | 8.1596       | 7.6275        | 2.2861          | 2.1306          |
Table 5: Energy gaps (eV) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial C atoms from 1 to 4. The values are reported for the lowest energy structures.

| X   | $E_{g}^{Si-bulk}$ | $E_{g}^{GB}$ | $E_{g}^{V1GB}$ | $E_{g}^{V2GB}$ |
|-----|------------------|--------------|----------------|--------------|
| 1C  | 0                | 0.0477       | 0.3587         | 0.4014       |
| 2C  | 0.4291           | 0.5235       | 0              | 0            |
| 3C  | 0.6944           | 0.4729       | 0.6066         | 0.5578       |
| 4C  | 0.4549           | 0.1319       | 0.6502         | 0.5978       |

Table 6: Hydrostatic pressure (GPa) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial C atoms from 1 to 4. The values are reported for the lowest energy structures.

| X   | $P(X+B)$ | $P(X+GB)$ | $P(X+V1GB)$ | $P(X+V2GB)$ |
|-----|----------|-----------|-------------|-------------|
| 1C  | 2.564    | 2.281     | 0.674       | 0.673       |
| 2C  | 3.850    | 2.756     | 1.507       | 1.502       |
| 3C  | 3.742    | 2.845     | 2.343       | 2.359       |
| 4C  | 4.734    | 3.356     | 2.563       | 2.543       |

2.2 Bonding analysis
| Si-Bulk | BC(Si-Si) | BL(Si-Si)Å | BC(Si-C) | BL(Si-C)Å | BC(C-C) | BL(C-C)Å | LP     |
|---------|-----------|------------|----------|-----------|---------|-----------|--------|
| 1C      | 1.9917    | 2.31736    | 2.4598   | 1.81289   |         |           | 0.14269|
|         | 1.9916    | 2.31759    | 2.5371   | 1.81233   |         |           |        |
|         | 1.9950    | 2.31807    | 2.3758   | 1.74694   |         |           |        |
|         | 1.9948    | 2.31842    |          |           |         |           |        |
|         | 2.2328    | 2.28068    |          |           |         |           |        |
|         | 2.2350    | 2.28173    |          |           |         |           |        |
|         | 1.9995    | 2.44675    |          |           |         |           |        |
| 2C      | 1.9779    | 2.31447    | 2.4845   | 1.78563   | 3.0651  | 1.31413   |        |
|         | 1.9781    | 2.31436    | 2.4843   | 1.78585   |         |           |        |
|         | 1.9779    | 2.31428    | 1.7554   | 1.84197   |         |           |        |
|         | 1.9782    | 2.31450    | 1.7557   | 1.84192   |         |           |        |
|         | 2.1463    | 2.25425    |          |           |         |           |        |
|         | 2.1460    | 2.25412    |          |           |         |           |        |
|         | 1.9930    | 2.30624    |          |           |         |           |        |
| 3C      | 2.0201    | 2.31590    | 2.3825   | 1.81499   | 1.5792  | 1.53572   |        |
|         | 2.0046    | 2.30954    | 2.3820   | 1.81535   |         | 1.5777    |        |
|         | 2.0047    | 2.30951    | 1.9941   | 1.87728   |         | 1.41599   | 1.50008|
|         | 2.0202    | 2.31584    | 1.9021   | 1.87268   |         |           |        |
|         | 2.0693    | 2.34550    | 1.9028   | 1.87244   |         |           |        |
|         | 2.0693    | 2.28066    |          |           |         |           |        |
|         | 2.1675    | 2.20866    |          |           |         |           |        |
|         | 1.9581    | 2.24297    |          |           |         |           |        |
|         | 1.9577    | 2.24290    |          |           |         |           |        |
| 4C      | 1.9954    | 2.36665    | 2.2361   | 1.84433   | 2.1508  | 1.41648   | 0.01604|
|         | 2.0178    | 2.32830    | 2.3127   | 1.80898   | 3.0399  | 1.34593   |        |
|         | 2.0250    | 2.38233    | 2.2938   | 1.85218   | 1.7943  | 1.46732   |        |
|         | 2.0650    | 2.26366    | 2.3754   | 1.81756   | 1.0551  | 1.66790   |        |
|         | 2.0407    | 2.28754    | 1.9845   | 1.86359   |         |           |        |
|         | 1.9946    | 2.30892    | 2.1936   | 1.87557   |         |           |        |
|         | 1.9880    | 2.31720    |          |           |         |           |        |
|         | 1.9545    | 2.34714    |          |           |         |           |        |
|         | 1.9410    | 2.35165    |          |           |         |           |        |

Table 7: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-C and C-C bonds with the inclusion of n numbers of C atoms (n=1,2,3 & 4) in Si-bulk.
| Si-GB | BC(Si-Si) | BL(Si-Si) Å | BC(Si-C) | BL(Si-C) Å | BC(C-C) | BL(C-C) Å | LP |
|-------|-----------|-------------|----------|------------|---------|-----------|----|
| 1C    | 1.9903    | 2.31786     | 2.2747   | 1.81425    |         |           | 0.5948 |
|       | 2.0164    | 2.31981     | 2.2497   | 1.81470    |         |           |      |
|       | 1.9814    | 2.31807     | 2.4034   | 1.74762    |         |           |      |
|       | 2.2083    | 2.29283     |         |            |         |           |      |
|       | 2.0041    | 2.33252     |         |            |         |           |      |
|       | 2.2183    | 2.29363     |         |            |         |           |      |
|       | 2.0015    | 2.45067     |         |            |         |           |      |
| 2C    | 2.0507    | 2.37415     | 2.3492   | 1.83840    | 2.8306  | 1.37792   |     |
|       | 2.0595    | 2.36930     | 2.3430   | 1.84499    |         |           |      |
|       | 2.0793    | 2.27725     | 2.1074   | 1.86866    |         |           |      |
|       | 2.0129    | 2.29788     | 2.1091   | 1.86785    |         |           |      |
|       | 2.0158    | 2.29966     |         |            |         |           |      |
|       | 1.9780    | 2.34655     |         |            |         |           |      |
|       | 1.9662    | 2.35109     |         |            |         |           |      |
|       | 2.0841    | 2.26822     |         |            |         |           |      |
|       | 2.0117    | 2.34787     |         |            |         |           |      |
|       | 1.9379    | 2.31357     |         |            |         |           |      |
| 3C    | 2.0549    | 2.42702     | 2.2420   | 1.85243    | 1.5274  | 1.57712   | C3: 0.001514 |
|       | 2.0493    | 2.30263     | 2.2603   | 1.85057    |         |           |      |
|       | 2.0167    | 2.33603     | 2.2152   | 1.84016    |         |           |      |
|       | 2.0128    | 2.33161     | 2.1312   | 1.85078    |         |           |      |
|       | 2.0341    | 2.35625     | 2.1595   | 1.84555    |         |           |      |
|       | 2.0395    | 2.32409     | 1.8675   | 1.93941    |         |           |      |
|       | 2.0554    | 2.44381     | 1.8601   | 1.93139    |         |           |      |
|       | 1.9637    | 2.32060     | 1.8795   | 1.88733    |         |           |      |
|       | 2.2222    | 2.21525     | 1.6191   | 1.88109    |         |           |      |
|       |           |             | 1.5615   | 1.89062    |         |           |      |
| 4C    | 2.0053    | 2.31422     | 2.3129   | 1.83722    | 2.5353  | 1.39499   |     |
|       | 2.0744    | 2.32324     | 2.2215   | 1.87488    |         |           |      |
|       | 2.0044    | 2.33814     | 2.1408   | 1.89536    |         |           |      |
|       | 2.0281    | 2.36433     | 2.4743   | 1.78531    |         |           |      |
|       | 1.9727    | 2.34566     | 2.4729   | 1.78473    |         |           |      |
|       | 1.9471    | 2.32925     | 2.4820   | 1.80381    |         |           |      |
|       | 1.8315    | 2.48968     | 2.5122   | 1.77339    |         |           |      |
|       | 1.8336    | 2.44290     | 2.1517   | 1.79929    |         |           |      |
|       | 1.1289    | 2.57283     | 2.7127   | 1.75854    |         |           |      |
|       |           |             | 1.7269   | 1.95371    |         |           |      |
|       |           |             | 1.1668   | 2.03012    |         |           |      |

Table 8: Bond charge (BC), bond length (BL) and lone pair (LP) data for Si-Si, Si-C and C-C bonds with the inclusion of n numbers of C atoms (n=1,2,3 & 4) in Si-GB
|     | BC(Si-Si) | BL(Si-Si)Å | BC(Si-C) | BL(Si-C)Å | BC(C-C) | BL(C-C)Å | LP    |
|-----|-----------|------------|----------|------------|----------|----------|-------|
| 1C  | 2.0243    | 2.39351    | 1.9629   | 1.99583    |          |          |       |
|     | 2.0242    | 2.39361    | 1.9526   | 2.00851    |          |          |       |
|     | 2.0205    | 2.39538    | 1.9201   | 2.03954    |          |          |       |
|     | 2.0289    | 2.39751    | 1.9199   | 2.03983    |          |          |       |
|     | 2.0210    | 2.40463    |          |            |          |          |       |
|     | 2.0211    | 2.40463    |          |            |          |          |       |
|     | 2.0291    | 2.39740    |          |            |          |          |       |
|     | 2.0115    | 2.34935    |          |            |          |          |       |
|     | 2.0237    | 2.40396    |          |            |          |          |       |
|     | 2.0115    | 2.34945    |          |            |          |          |       |
|     | 2.0238    | 2.40392    |          |            |          |          |       |
|     | 1.9847    | 2.34152    |          |            |          |          |       |
|     | 2.0026    | 2.46212    |          |            |          |          |       |
|     | 1.9689    | 2.42414    |          |            |          |          |       |
| V1  | 2.0236    | 2.40835    | 2.4013   | 1.88745    | 2.3241   | 1.41529  |       |
|     | 2.0234    | 2.42022    | 2.4174   | 1.88984    |          |          |       |
|     | 2.0299    | 2.42408    | 2.4146   | 1.88913    |          |          |       |
|     | 2.0176    | 2.42635    | 2.4217   | 1.88409    |          |          |       |
|     | 2.0019    | 2.33929    |          |            |          |          |       |
|     | 2.0023    | 2.34743    |          |            |          |          |       |
|     | 2.0037    | 2.34256    |          |            |          |          |       |
|     | 1.9859    | 2.37766    |          |            |          |          |       |
|     | 1.9560    | 2.37192    |          |            |          |          |       |
|     | 1.9545    | 2.37375    |          |            |          |          |       |
| 3C  | 2.0355    | 2.32286    | 2.6560   | 1.80175    | 3.0039   | 1.31195  |       |
|     | 2.0148    | 2.39841    | 2.7033   | 1.80450    | 1.5660   | 1.51629  |       |
|     | 2.0329    | 2.29982    | 2.1869   | 1.89111    | 1.5181   | 1.52702  |       |
|     | 2.0273    | 2.33162    | 2.1780   | 1.90020    |          |          |       |
|     | 2.0332    | 2.32608    |          |            |          |          |       |
|     | 1.9774    | 2.32650    |          |            |          |          |       |
|     | 1.9799    | 2.34479    |          |            |          |          |       |
|     | 1.9779    | 2.34151    |          |            |          |          |       |
|     | 2.0099    | 2.42987    |          |            |          |          |       |
|     | 1.9848    | 2.31307    |          |            |          |          |       |
|     | 1.9863    | 2.37639    |          |            |          |          |       |
|     | 1.9979    | 2.37766    |          |            |          |          |       |
|     | 1.9875    | 2.37762    |          |            |          |          |       |
| 4C  | 2.0668    | 2.30703    | 2.3035   | 1.85418    | 1.6203   | 1.53713  | C1: 0.010741 |
|     | 2.0139    | 2.31936    | 2.5360   | 1.83508    | 1.6193   | 1.53703  | C3: 0.035845 |
|     | 2.0058    | 2.34112    | 2.5114   | 1.83507    | 1.5869   | 1.55733  | C3: 0.021072 |
|     | 2.0131    | 2.34511    | 2.3171   | 1.85991    | 1.5648   | 1.55739  |       |
|     | 2.0274    | 2.37703    | 2.0619   | 1.84544    | 1.3678   | 1.46903  |       |
|     | 2.0276    | 2.37684    | 2.0494   | 1.90386    |          |          |       |
|     | 2.0429    | 2.35443    |          |            |          |          |       |
|     | 2.0429    | 2.35446    |          |            |          |          |       |
|     | 2.0115    | 2.29645    |          |            |          |          |       |
|     | 2.0414    | 2.36713    |          |            |          |          |       |

Table 9: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-C and C-C bonds with the inclusion of n numbers of C atoms (n=1,2,3 & 4) in Si-GB with vacancy V1.
| Si-VGB | BC(Si-Si) | BL(Si-Si) A | BC(Si-C) | BL(Si-C) A | BC(C-C) | BL(C-C) A | LP |
|--------|-----------|-------------|----------|-------------|---------|------------|-----|
| 1C     | 2.0281    | 2.38089     | 1.9623   | 2.00709     |         |            |     |
|        | 2.0281    | 2.38089     | 1.9271   | 2.01777     |         |            |     |
|        | 2.0184    | 2.38908     | 1.9333   | 2.03516     |         |            |     |
|        | 2.0207    | 2.40451     | 1.9333   | 2.03516     |         |            |     |
|        | 2.0207    | 2.40451     | 1.9333   | 2.03516     |         |            |     |
|        | 2.0272    | 2.39927     |         |             |         |            |     |
|        | 2.0272    | 2.39927     |         |             |         |            |     |
|        | 2.0224    | 2.39941     |         |             |         |            |     |
|        | 2.0016    | 2.39996     |         |             |         |            |     |
|        | 2.0022    | 2.46209     |         |             |         |            |     |
|        | 2.0022    | 2.46209     |         |             |         |            |     |
| V2     | 2.0119    | 2.32572     | 2.3918   | 1.89263     | 2.3152  | 1.41603    |     |
|        | 2.0235    | 2.40835     | 2.4065   | 1.89224     |         |            |     |
|        | 2.0171    | 2.42459     | 2.4949   | 1.87145     |         |            |     |
|        | 2.0034    | 2.32550     | 2.4071   | 1.88101     |         |            |     |
|        | 1.9984    | 2.38682     |         |             |         |            |     |
|        | 1.9612    | 2.35986     |         |             |         |            |     |
|        | 1.9912    | 2.33270     |         |             |         |            |     |
|        | 1.9641    | 2.41901     |         |             |         |            |     |
|        | 1.9530    | 2.37274     |         |             |         |            |     |
|        | 1.9518    | 2.37180     |         |             |         |            |     |
| 3C     | 2.0037    | 2.33228     | 2.6418   | 1.80187     | 2.9989  | 1.31248    |     |
|        | 1.9961    | 2.33392     | 2.7338   | 1.79859     | 1.5669  | 1.51368    |     |
|        | 1.9890    | 2.33664     | 2.1864   | 1.89848     | 1.5185  | 1.52813    |     |
|        | 2.0321    | 2.30156     | 2.1773   | 1.90683     |         |            |     |
|        | 2.0308    | 2.33111     |         |             |         |            |     |
|        | 2.0230    | 2.32828     |         |             |         |            |     |
|        | 2.0121    | 2.41445     |         |             |         |            |     |
|        | 2.0278    | 2.32947     |         |             |         |            |     |
| 4C     | 2.0689    | 2.31040     | 2.2894   | 1.86170     | 1.6442  | 1.53314    |     |
|        | 2.0040    | 2.33369     | 2.5498   | 1.83354     | 1.6105  | 1.53866    |     |
|        | 1.9870    | 2.32764     | 2.5521   | 1.84761     | 1.5948  | 1.55655    |     |
|        | 2.0023    | 2.33598     | 2.3272   | 1.86247     | 1.5870  | 1.55328    |     |
|        | 2.0042    | 2.33820     | 2.0410   | 1.84755     | 1.3498  | 1.47835    |     |
|        | 2.0345    | 2.35649     | 2.0608   | 1.90940     |         |            |     |

Table 10: Bond charge (BC), bond length (BL) and lone pair (LP) data for Si-Si, Si-C and C-C bonds with the inclusion of n numbers of C atoms (n=1,2,3 & 4) in Si-GB with vacancy V2.
3 Systems with interstitial nitrogen impurities

3.1 Electronic properties

|   | $E_{\text{Si}}$ | $E_{\text{SiGB}}$ | $E_{\text{V1GB}}$ | $E_{\text{V2GB}}$ |
|---|-----------------|-------------------|-------------------|-------------------|
| 1N | 1.8155          | 1.3127            | -0.8477           | -1.8618           |
| 2N | -0.7577         | -0.9272           | -1.5182           | -2.4698           |
| 3N | 0.5968          | -0.4488           | -1.8968           | -2.0912           |
| 4N | 1.2163          | -1.5700           | -3.0445           | -4.1177           |

Table 11: Formation energy (eV) of Si bulk and $\Sigma3\{111\}$ Si GB without/with vacancies V1 and V2 with interstitial N atoms from 1 to 4. The values are reported for the lowest energy structures.

|   | $E_{\text{Si-bulk}}$ | $E_{\text{SiGB}}$ | $E_{\text{V1GB}}$ | $E_{\text{V2GB}}$ |
|---|----------------------|-------------------|-------------------|-------------------|
| 1N | 0                    | 0                 | 0                 | 0                 |
| 2N | 0.5427               | 0.5444            | 0.2439            | 0.6191            |
| 3N | 0                    | 0                 | 0                 | 0                 |
| 4N | 0.3464               | 0.6274            | 0.3966            | 0.6397            |

Table 12: Energy gaps (eV) of Si bulk and $\Sigma3\{111\}$ Si GB without/with vacancies V1 and V2 with interstitial N atoms from 1 to 4. The values are reported for the lowest energy structures.

|   | $P_{\text{X+B}}$ | $P_{\text{X+GB}}$ | $P_{\text{X+V1GB}}$ | $P_{\text{X+V2GB}}$ |
|---|------------------|-------------------|-------------------|-------------------|
| 1N | 2.682            | 2.027             | 1.601             | 0.867             |
| 2N | 2.959            | 2.577             | 1.275             | 0.820             |
| 3N | 3.161            | 2.850             | 1.054             | 1.327             |
| 4N | 3.464            | 3.017             | 1.331             | 1.376             |

Table 13: Hydrostatic pressure (GPa) of Si bulk and $\Sigma3\{111\}$ Si GB without/with vacancies V1 and V2 with interstitial N atoms from 1 to 4. The values are reported for the lowest energy structures.

3.2 Bonding analysis
| Si-Bulk | BC(Si-Si) | BL(Si-Si)Å | BC(Si-N) | BL(Si-N)Å | BC(N-N) | BL(N-N)Å | LP       |
|---------|-----------|------------|----------|-----------|---------|----------|----------|
| 1N      | 2.0478    | 2.33613    | 2.4274   | 1.66719   |         |          | 2.4509   |
|         | 1.9314    | 2.32035    | 2.4114   | 1.66703   |         |          |          |
|         | 1.9270    | 2.32165    |          |           |         |          |          |
|         | 2.0029    | 2.35253    |          |           |         |          |          |
|         | 2.0013    | 2.35318    |          |           |         |          |          |
|         | 2.0181    | 2.35985    |          |           |         |          |          |
|         | 1.9412    | 2.33676    |          |           |         |          |          |
|         | 1.9427    | 2.33660    |          |           |         |          |          |
| 2N      | 2.0849    | 2.30713    | 2.2752   | 1.73464   |         |          | N1: 1.4121|
|         | 2.0843    | 2.30644    | 2.2956   | 1.73455   |         |          | N2: 1.3700|
|         | 2.0843    | 2.30645    | 2.0008   | 1.73999   |         |          |          |
|         | 2.0849    | 2.30701    | 2.0007   | 1.73986   |         |          |          |
|         | 2.0244    | 2.31767    | 2.0293   | 1.76801   |         |          |          |
|         | 2.0239    | 2.31746    | 2.0508   | 1.76801   |         |          |          |
| 3N      | 2.0352    | 2.28999    | 2.2909   | 1.73687   |         |          | N1: 0.7259|
|         | 2.0792    | 2.30490    | 2.3008   | 1.73777   |         |          | N2: 0.8651|
|         | 2.0869    | 2.31795    | 1.9742   | 1.74611   |         |          | N3: 1.9743|
|         | 2.0827    | 2.33198    | 2.0136   | 1.74460   |         |          |          |
|         | 2.0912    | 2.30624    | 1.9209   | 1.76536   |         |          |          |
|         | 2.0617    | 2.28782    | 2.1595   | 1.76647   |         |          |          |
|         | 2.0273    | 2.31692    | 1.8634   | 1.73632   |         |          |          |
|         | 2.0109    | 2.31369    | 2.0166   | 1.76668   |         |          |          |
|         |           |            | 1.8249   | 1.78669   |         |          |          |
| 4N      | 2.0829    | 2.33553    | 2.3121   | 1.73744   |         |          | N1: 1.2854|
|         | 2.0801    | 2.32301    | 2.3443   | 1.71281   |         |          | N2: 1.3015|
|         | 2.0871    | 2.29693    | 2.0021   | 1.75323   |         |          | N3: 1.5256|
|         | 2.1036    | 2.30566    | 2.0234   | 1.74916   |         |          | N4: 1.9553|
|         | 2.1494    | 2.25315    | 1.9686   | 1.75665   |         |          |          |
|         | 2.1334    | 2.35389    | 1.9389   | 1.77627   |         |          |          |
|         | 1.9851    | 2.30198    | 2.2747   | 1.72530   |         |          |          |
|         |           |            | 1.9527   | 1.74615   |         |          |          |
|         |           |            | 2.0948   | 1.76061   |         |          |          |
|         |           |            | 2.0943   | 1.77118   |         |          |          |
|         |           |            | 1.9726   | 1.73255   |         |          |          |
|         |           |            | 1.7351   | 1.76306   |         |          |          |

Table 14: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-N and N-N bonds with the inclusion of n numbers of N atoms (n=1,2,3 & 4) in Si-bulk.
| Si-GB | BC(Si-Si) | BL(Si-Si)Å | BC(Si-N) | BL(Si-N)Å | BC(N-N) | BL(N-N)Å | LP       |
|-------|-----------|------------|----------|-----------|----------|-----------|----------|
| 1N    | 2.0376    | 2.32647    | 2.0010   | 1.76298   | 1.9985   | 2.0375    | 2.32636  | 2.0000   | 1.76189   | 1.9985   | 2.0492    | 2.32064  | 2.1552   | 1.76611   | 1.9985   | 2.0493    | 2.32045  | 1.9200   | 1.76417   | 1.9985   | 2.0331    | 2.45711  | 1.7552   | 1.76386   | 1.9985   | 2.1035    | 2.31514  | 1.9200   | 1.7552    | 1.9985   | 2.1035    | 2.31462  | 1.7552   | 1.76386   | 1.9985   | 2.0271    | 2.43737  | 1.9200   | 1.7552    | 1.9985   | 1.9985   | 2.0271    | 2.43737  | 1.9200   | 1.7552    | 1.9985   | 2.0271    | 2.43737  | 1.9200   | 1.7552    | 1.9985   | 2.0271    | 2.43737  |
| 2N    | 2.0834    | 2.3185     | 2.3180   | 1.73044   | 2.0492    | 2.32064  | 2.3180   | 1.73044   | 2.0492    | 2.32064  | 2.3180   | 1.73044   | 2.0493    | 2.32045  | 1.9200   | 1.76417   | 1.9985   | 2.0493    | 2.32045  | 1.9200   | 1.76417   | 1.9985   | 2.0331    | 2.45711  | 1.7552   | 1.76386   | 1.9985   | 2.1035    | 2.31514  | 1.9200   | 1.7552    | 1.9985   | 2.1035    | 2.31462  | 1.9200   | 1.7552    | 1.9985   | 2.0271    | 2.43737  | 1.9200   | 1.7552    | 1.9985   | 1.9985   |
| 3N    | 2.1013    | 2.29004    | 2.1939   | 1.74968   | 2.0492    | 2.32064  | 2.1939   | 1.74968   | 2.0492    | 2.32064  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   | 1.74968   | 2.0493    | 2.32045  | 2.1939   |
| 4N    | 2.1249    | 2.27680    | 2.4731   | 1.73868   | 2.0492    | 2.32064  | 2.4731   | 1.73868   | 2.0492    | 2.32064  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   | 1.73868   | 2.0493    | 2.32045  | 2.4731   |

Table 15: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-N and N-N bonds with the inclusion of n numbers of N atoms (n=1,2,3 & 4) in Si-GB.
|   | Si-VGB | BC(Si-Si) | BL(Si-Si)Å | BC(Si-N) | BL(Si-N)Å | BC(N-N) | BL(N-N)Å | LP  |
|---|--------|-----------|------------|----------|------------|----------|-----------|-----|
| 1N |        | 2.0247    | 2.41953    | 2.3100   | 1.69449    |          |           | 2.9121|
|    |        | 2.0197    | 2.43623    | 2.2639   | 1.69582    |          |           |      |
|    |        | 2.0010    | 2.35263    |          |            |          |           |      |
|    |        | 2.0038    | 2.34135    |          |            |          |           |      |
|    |        | 2.0009    | 2.35266    |          |            |          |           |      |
|    |        | 1.9653    | 2.38943    |          |            |          |           |      |
|    |        | 1.9649    | 2.38938    |          |            |          |           |      |
|    |        | 2.0462    | 2.30787    |          |            |          |           |      |
|    |        | 1.9577    | 2.38419    |          |            |          |           |      |
|    |        | 1.9570    | 2.38426    |          |            |          |           |      |
|    |        | 2.0887    | 2.32091    |          |            |          |           |      |
|    |        | 2.0894    | 2.31500    |          |            |          |           |      |
|    |        | 1.9718    | 2.30958    |          |            |          |           |      |
|   | V1     | 2.0434    | 2.34686    | 1.70999  | 1.80391    |          | 1.0824   | 1.45049|
|    |        | 2.0256    | 2.41936    | 1.6528   | 1.80577    |          |          |      |
|    |        | 2.0453    | 2.34935    | 1.5105   | 1.83934    |          |          |      |
|    |        | 2.0452    | 2.34960    | 1.5587   | 1.83902    |          |          |      |
|    |        | 2.0501    | 2.33689    |          |            |          |           |      |
|    |        | 2.0484    | 2.35730    |          |            |          |           |      |
|    |        | 2.0241    | 2.44403    |          |            |          |           |      |
|    |        | 2.0094    | 2.34903    |          |            |          |           |      |
|    |        | 1.9838    | 2.33999    |          |            |          |           |      |
|    |        | 1.9960    | 2.55257    |          |            |          |           |      |
|   | 2N     | 2.0773    | 2.41155    | 2.3000   | 1.73292    |          |          |      |
|    |        | 2.0422    | 2.37194    | 1.9799   | 1.82098    |          |          |      |
|    |        | 2.0225    | 2.33420    | 1.9268   | 1.78660    |          |          |      |
|    |        | 2.0439    | 2.40624    | 2.3839   | 1.68197    |          |          |      |
|    |        | 1.9813    | 2.31695    | 1.9969   | 1.79269    |          |          |      |
|    |        | 2.0262    | 2.37227    | 2.3275   | 1.70177    |          |          |      |
|    |        | 2.0281    | 2.42340    | 1.9324   | 1.81505    |          |          |      |
|    |        | 2.0372    | 2.40966    | 1.7521   | 1.84096    |          |          |      |
|    |        | 2.0574    | 2.48591    |          |            |          |           |      |
|   | 3N     | 2.1485    | 2.46424    | 2.0854   | 1.74349    |          |          |      |
|    |        | 2.0467    | 2.35171    | 2.0270   | 1.73643    |          |          |      |
|    |        | 2.0365    | 2.42135    | 2.0928   | 1.77086    |          |          |      |
|    |        | 2.0349    | 2.38921    | 2.1196   | 1.75251    |          |          |      |
|    |        | 2.0348    | 2.41911    | 1.9919   | 1.77712    |          |          |      |
|    |        | 2.0138    | 2.36413    | 2.0611   | 1.79525    |          |          |      |
|    |        | 1.9812    | 2.32272    | 2.0450   | 1.79535    |          |          |      |
|    |        | 2.0344    | 2.49119    | 1.8110   | 1.76966    |          |          |      |
|    |        |           |           | 2.2998   | 1.80866    |          |          |      |
|    |        |           |           | 1.8331   | 1.84124    |          |          |      |
|    |        |           |           | 2.3149   | 1.77682    |          |          |      |
|    |        |           |           | 1.6849   | 1.80845    |          |          |      |
|   | 4N     | 2.2998    | 1.80866    |          |            |          |           |      |
|    |        | 2.1852    | 1.2873     |          |            |          |           |      |
|    |        | 1.2731    | 1.2097     |          |            |          |           |      |

Table 16: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-N and N-N bonds with the inclusion of n numbers of N atoms (n=1,2,3 & 4) in Si-GB with vacancy V1.
|          | Si-VGB | BC(Si-Si) | BL(Si-Si)Å | BC(Si-N) | BL(Si-N)Å | BC(N-N) | BL(N-N)Å | LP       |
|----------|--------|-----------|------------|----------|-----------|---------|----------|----------|
| 1N       |        |           |            |          |           |         |          |          |
|          | 2.0564 | 2.36784   | 1.9553     | 1.87247  |           |         |          | N: 1.6904 |
|          | 2.0509 | 2.40413   | 1.9558     | 1.87367  |           |         |          | Si: 0.4432 |
|          | 2.0493 | 2.40528   | 1.9353     | 1.86030  |           |         |          |          |
|          | 2.0511 | 2.38624   | 1.9353     | 1.86030  |           |         |          |          |
|          | 2.0483 | 2.38886   | 1.9353     | 1.86030  |           |         |          |          |
|          | 1.9908 | 2.40434   | 1.9353     | 1.86030  |           |         |          |          |
|          | 1.9654 | 2.40723   | 1.9353     | 1.86030  |           |         |          |          |
|          | 2.1537 | 2.33401   | 1.9353     | 1.86030  |           |         |          |          |
|          | 2.1767 | 2.33784   | 1.9353     | 1.86030  |           |         |          |          |
|          | 2.2444 | 2.32922   | 1.9353     | 1.86030  |           |         |          |          |
| V2       |        |           |            |          |           |         |          |          |
| 2N       |        |           |            |          |           |         |          |          |
|          | 2.0061 | 2.31947   | 2.0590     | 1.76352  |           |         |          | N1: 1.8892 |
|          | 2.0063 | 2.31967   | 2.0490     | 1.76331  |           |         |          | N2: 1.9015 |
|          | 2.0476 | 2.36605   | 1.9409     | 1.80508  |           |         |          |          |
|          | 2.0227 | 2.33318   | 1.9121     | 1.80526  |           |         |          |          |
|          | 2.0426 | 2.45558   | 1.7975     | 1.82537  |           |         |          |          |
|          | 2.0550 | 2.53332   | 1.7913     | 1.82514  |           |         |          |          |
|          | 2.0549 | 2.53382   | 1.7913     | 1.82514  |           |         |          |          |
| 3N       |        |           |            |          |           |         |          |          |
|          | 2.0252 | 2.36235   | 2.4391     | 1.75975  |           |         |          | N1: 1.2519 |
|          | 2.0156 | 2.33604   | 1.9526     | 1.77458  |           |         |          | N2: 2.1413 |
|          | 2.0422 | 2.35106   | 2.7003     | 1.65230  |           |         |          | N3: 2.1548 |
|          | 2.0451 | 2.35443   | 1.9947     | 1.77620  |           |         |          |          |
|          | 2.0241 | 2.38609   | 2.0178     | 1.78340  |           |         |          |          |
|          | 2.0507 | 2.43521   | 2.5160     | 1.66644  |           |         |          |          |
|          | 2.0473 | 2.41717   | 1.8130     | 1.79287  |           |         |          |          |
|          | 2.0488 | 2.51035   | 1.7839     | 1.81480  |           |         |          |          |
|          | 2.0415 | 2.51595   | 1.7839     | 1.81480  |           |         |          |          |
|          | 1.7991 | 2.35569   |            |          |           |         |          |          |
| 4N       |        |           |            |          |           |         |          |          |
|          | 2.0319 | 2.28568   | 2.2734     | 1.73678  |           |         |          | N1: 1.8719 |
|          | 2.1039 | 2.42680   | 2.1041     | 1.75573  |           |         |          | N2: 1.3477 |
|          | 2.0438 | 2.26015   | 2.1349     | 1.76866  |           |         |          | N3: 1.2853 |
|          | 2.0431 | 2.35302   | 2.0410     | 1.74235  |           |         |          | N4: 2.0208 |
|          | 2.0439 | 2.35439   | 2.4054     | 1.75972  |           |         |          |          |
|          | 2.0269 | 2.37705   | 1.9884     | 1.77301  |           |         |          |          |
|          | 1.9962 | 2.33643   | 2.0737     | 1.76081  |           |         |          |          |
|          | 2.0385 | 2.42899   | 1.9729     | 1.78870  |           |         |          |          |
|          | 2.0439 | 2.42410   | 1.8965     | 1.77478  |           |         |          |          |
|          | 2.0702 | 2.47255   | 1.9491     | 1.77956  |           |         |          |          |
|          | 2.0709 | 2.51903   | 1.8610     | 1.79077  |           |         |          |          |
|          | 2.0000 | 2.46747   | 1.7530     | 1.80498  |           |         |          |          |

Table 17: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-N and N-N bonds with the inclusion of n numbers of N atoms (n=1,2,3 & 4) in Si-GB with vacancy V2.
4 Systems with interstitial oxygen impurities

4.1 Electronic properties

| X  | $E_i^{\text{Si-bulk}}$ | $E_i^{\text{GB}}$ | $E_i^{\text{V1GB}}$ | $E_i^{\text{V2GB}}$ |
|----|------------------------|-------------------|-------------------|-------------------|
| 1O | -2.3649                | -2.3950           | -4.3281           | -4.3036          |
| 2O | -5.2126                | -5.2515           | -7.9224           | -7.8855          |
| 3O | -8.3195                | -8.3974           | -11.2368          | -11.2213         |
| 4O | -11.0994               | -11.1843          | -14.2579          | -14.5924         |

Table 18: Formation energy (eV) of Si bulk and $\Sigma3\{111\}$ Si GB without/with vacancies V1 and V2 with interstitial O atoms from 1 to 4. The values are reported for the lowest energy structures.

| X  | $E_g^{\text{Si-bulk}}$ | $E_g^{\text{GB}}$ | $E_g^{\text{V1GB}}$ | $E_g^{\text{V2GB}}$ |
|----|------------------------|-------------------|-------------------|-------------------|
| 1O | 0.6086                 | 0.5506            | 0.6274            | 0.6283            |
| 2O | 0.5913                 | 0.6073            | 0.6353            | 0.6292            |
| 3O | 0.7285                 | 0.6185            | 0.6306            | 0.6319            |
| 4O | 0.7430                 | 0.5569            | 0.6850            | 0.6989            |

Table 19: Energy gaps (eV) of Si bulk and $\Sigma3\{111\}$ Si GB with/without vacancies V1 and V2 with interstitial O atoms from 1 to 4. The values are reported for the lowest energy structures.

| X  | $P(X+B)$ | $P(X+\text{GB})$ | $P(X+V1\text{GB})$ | $P(X+V2\text{GB})$ |
|----|----------|------------------|-------------------|-------------------|
| 1O | 2.776    | 2.413            | 1.697             | 1.692             |
| 2O | 3.157    | 2.660            | 2.325             | 2.282             |
| 3O | 3.479    | 2.864            | 2.981             | 2.616             |
| 4O | 4.121    | 3.064            | 3.171             | 2.849             |

Table 20: Hydrostatic pressure (GPa) of Si bulk and $\Sigma3\{111\}$ Si GB without/with vacancies V1 and V2 with interstitial O atoms from 1 to 4. The values are reported for the lowest energy structures.

4.2 Bonding analysis
Table 21: Bond charge (BC), bond length (BL) and lone pair (LP) data for Si-Si and Si-O bonds with the inclusion of n numbers of O atoms (n=1,2,3 & 4) in Si-bulk.

| Si-Bulk | BC(Si-Si) | BL(Si-Si)Å | BC(Si-O) | BL(Si-O)Å | LP |
|---------|-----------|------------|----------|-----------|----|
| 1O      | 1.9918    | 2.32115    | 1.7489   | 1.63550   | O1: 4.283 |
|         | 2.0069    | 2.32194    | 1.7479   | 1.63423   |    |
|         | 2.0467    | 2.32461    |          |           |    |
|         | 2.0555    | 2.32523    |          |           |    |
| 2O      | 2.0789    | 2.30065    | 1.8939   | 1.64273   | O1: 4.2801 |
|         | 2.0795    | 2.30074    | 1.7391   | 1.66098   | O2: 4.3145 |
|         | 2.0221    | 2.32101    | 1.7493   | 1.63986   |    |
|         | 1.9685    | 2.31220    | 1.5902   | 1.67594   |    |
|         | 2.0680    | 2.33876    |          |           |    |
|         | 2.0681    | 2.33886    |          |           |    |
|         | 2.0950    | 2.33589    |          |           |    |
| 3O      | 2.1373    | 2.24814    | 1.9606   | 1.62698   | O1: 4.3299 |
|         | 1.9904    | 2.30827    | 1.9473   | 1.62684   | O2: 4.3404 |
|         | 2.0606    | 2.33173    | 1.9752   | 1.62684   | O3: 4.3299 |
|         | 2.0602    | 2.33169    | 1.5148   | 1.68729   |    |
|         | 2.0598    | 2.33175    | 1.5429   | 1.68740   |    |
|         | 2.0714    | 2.35013    | 1.5191   | 1.68737   |    |
|         | 2.0710    | 2.34967    |          |           |    |
| 4O      | 2.0971    | 2.22921    | 1.9675   | 1.63190   | O1: 4.2585 |
|         | 2.0108    | 2.32069    | 1.9450   | 1.62957   | O2: 4.1269 |
|         | 2.0322    | 2.32228    | 1.9281   | 1.62211   | O3: 4.2659 |
|         | 1.9837    | 2.30422    | 1.7651   | 1.66014   | O4: 4.3555 |
|         | 2.0497    | 2.33004    | 1.7301   | 1.63470   |    |
|         | 2.0734    | 2.34109    | 1.7331   | 1.65317   |    |
|         |           |            | 1.6537   | 1.66647   |    |
|         |           |            | 1.5824   | 1.68762   |    |
| Si-GB | BC(Si-Si) | BL(Si-Si) Å | BC(Si-O) | BL(Si-O) Å | LP |
|-------|-----------|-------------|-----------|-------------|----|
| 1O    | 2.0093    | 2.32532     | 1.7792    | 1.63913     | 4.2934 |
|       | 1.9902    | 2.32383     | 1.7035    | 1.63789     |    |
|       | 2.0134    | 2.33911     |          |             |    |
|       | 2.0425    | 2.32990     |          |             |    |
|       | 2.0564    | 2.32204     |          |             |    |
|       | 2.0781    | 2.32612     |          |             |    |
|       | 1.9997    | 2.32640     |          |             |    |
|       | 1.9931    | 2.34696     |          |             |    |
|       | 1.9959    | 2.36746     |          |             |    |
| 2O    | 2.0872    | 2.31206     | 1.9142    | 1.64514     | O1: 4.3003 |
|       | 2.0250    | 2.32108     | 1.7951    | 1.64091     | O2: 4.3380 |
|       | 2.0197    | 2.32159     | 1.7078    | 1.66111     |    |
|       | 2.0920    | 2.31034     | 1.5149    | 1.67498     |    |
|       | 2.0950    | 2.33289     |          |             |    |
|       | 2.0132    | 2.35452     |          |             |    |
|       | 2.0226    | 2.32704     |          |             |    |
|       | 1.9877    | 2.36383     |          |             |    |
|       | 1.9847    | 2.32704     |          |             |    |
|       | 1.9957    | 2.35741     |          |             |    |
| 3O    | 2.1448    | 2.25427     | 1.9600    | 1.62934     | O1: 4.2309 |
|       | 2.1231    | 2.28737     | 2.0395    | 1.62583     | O2: 4.3284 |
|       | 2.0699    | 2.34079     | 1.9255    | 1.63628     | O3: 4.3491 |
|       | 2.0687    | 2.36253     | 1.5670    | 1.68212     |    |
|       | 2.0445    | 2.33292     | 1.5497    | 1.68240     |    |
|       | 2.0624    | 2.34653     | 1.5057    | 1.69960     |    |
|       | 1.9502    | 2.32814     |          |             |    |
|       | 1.9914    | 2.33156     |          |             |    |
|       | 1.9873    | 2.33906     |          |             |    |
| 4O    | 1.9968    | 2.30098     | 2.1162    | 1.60775     | O1: 4.1798 |
|       | 2.0109    | 2.31141     | 1.9557    | 1.60825     | O2: 4.3162 |
|       | 2.0089    | 2.29839     | 2.0040    | 1.60321     | O3: 4.4751 |
|       | 2.0324    | 2.32370     | 1.9907    | 1.61242     | O4: 4.3444 |
|       | 2.0459    | 2.36708     | 1.5109    | 1.69476     |    |
|       | 2.0352    | 2.32384     | 1.5546    | 1.69474     |    |
|       | 2.0739    | 2.37431     | 1.5502    | 1.69645     |    |
|       | 2.1489    | 2.29031     | 1.4290    | 1.71093     |    |
|       | 1.9766    | 2.33417     |          |             |    |

Table 22: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si and Si-O bonds with the inclusion of n numbers of O atoms (n=1,2,3 & 4) in Si-GB
Table 23: Bond charge (BC), bond length (BL) and lone pair (LP) data for Si-Si and Si-O bonds with the inclusion of n numbers of O atoms (n=1,2,3 & 4) in Si-GB with vacancy V1.
Table 24: Bond charge (BC), bond length (BL) and lone pair (LP) data for Si-Si and Si-O bonds for the inclusion of n numbers of O atoms (n=1, 2, 3 & 4) in Si-GB with vacancy V2.
5 Bond charge variations

5.1 Nitrogen

Figure 2: Bond charge variation of Si-Si and Si-N with the inclusion of one nitrogen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond charges from bulk phases of Si and Si$_3$N$_4$ are marked in the inset of respective plots.
Figure 3: Bond charge variation of Si-Si, Si-N and N-N for the inclusion of two nitrogen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond charges from bulk phases of Si and Si$_3$N$_4$ are marked in the inset of respective plots.
Figure 4: Bond charge variation of Si-Si and Si-N for the inclusion of three nitrogen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond charges from bulk phases of Si and Si$_3$N$_4$ are marked in the inset of respective plots.
Figure 5: Bond charge variation of Si-Si and Si-N for the inclusion of four nitrogen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond charges from bulk phases of Si and Si$_3$N$_4$ are marked in the inset of respective plots.
5.2 Oxygen

Figure 6: Bond charge variation of Si-Si and Si-O for the inclusion of one oxygen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond charges from bulk phases of Si and SiO$_2$ are marked in the inset of respective plots.
Figure 7: Bond charge variation of Si-Si and Si-O for the inclusion of two oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond charges from bulk phases of Si and SiO$_2$ are marked in the inset of respective plots.
Figure 8: Bond charge variation of Si-Si and Si-O for the inclusion of three oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond charges from bulk phases of Si and SiO$_2$ are marked in the inset of respective plots.
Figure 9: Bond charge variation of Si-Si and Si-O for the inclusion of four oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond charges from bulk phases of Si and SiO$_2$ are marked in the inset of respective plots.
6  Bond length variations

6.1  Carbon

Figure 10: Bond length variation of Si-Si, Si-C and C-C for the inclusion of two carbon atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-C/C-C bond length from bulk phases of Si, SiC, diamond and molecular systems ethylene and ethane are marked in the inset of respective plots.
Figure 11: Bond length variation of Si-Si, Si-C and C-C for the inclusion of three carbon atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-C/C-C bond length from bulk phases of Si, SiC, diamond and molecular systems ethylene, ethane, and cyclopropene are marked in the inset of respective plots.
Figure 12: Bond length variation of Si-Si, Si-C and C-C for the inclusion of four carbon atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-C/C-C bond length from bulk phases of Si, SiC, diamond and molecular systems ethylene, ethane, and bicyclobutane are marked in the inset of respective plots.

6.2 Nitrogen
Figure 13: Bond length variation of Si-Si and Si-N for the inclusion of one nitrogen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond length from bulk phases of Si, Si$_3$N$_4$ are marked in the inset of respective plots.
Figure 14: Bond length variation of Si-Si, Si-N and N-N for the inclusion of two nitrogen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond length from bulk phases of Si, Si$_3$N$_4$ are marked in the inset of respective plots.
Figure 15: Bond length variation of Si-Si and Si-N for the inclusion of three nitrogen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond length from bulk phases of Si, Si$_3$N$_4$ are marked in the inset of respective plots.
Figure 16: Bond length variation of Si-Si and Si-N for the inclusion of four nitrogen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond length from bulk phases of Si, Si₃N₄ are marked in the inset of respective plots.
6.3 Oxygen

Figure 17: Bond length variation of Si-Si and Si-O for the inclusion of one oxygen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond length from bulk phases of Si, SiO$_2$ are marked in the inset of respective plots.
Figure 18: Bond length variation of Si-Si and Si-O for the inclusion of two oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond length from bulk phases of Si, SiO$_2$ are marked in the inset of respective plots.
Figure 19: Bond length variation of Si-Si and Si-O for the inclusion of three oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond length from bulk phases of Si, SiO₂ are marked in the inset of respective plots.
Figure 20: Bond length variation of Si-Si and Si-O for the inclusion of four oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond length from bulk phases of Si, SiO$_2$ are marked in the inset of respective plots.