

Results for forces and stress in SWSiCNT with Al-doped at Si site

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# Item: 0
# File: G:/SiC-Al-Ga/Tot_EN-STRESS-Forces-LSDA-SiCNT-(6.0)-1Al(Si).hdf5
# Title: Tot_EN-STRESS-Forces-LSDA-SiCNT-(6.0)-1Al(Si).hdf5 - Forces_0
# Type: Forces
+-----+
| Forces Report |
+-----+
| Index Element Force (eV/Ang) |
| x y z magnitude |
+-----+
| 0 Si -0.01905 -0.01384 -0.00833 0.02498 |
| 1 C 0.00357 -0.00005 0.00661 0.00751 |
| 2 C -0.00312 0.00853 0.00453 0.01015 |
| 3 Si -0.02075 0.00627 -0.00192 0.02177 |
| 4 C -0.00151 0.02276 0.01014 0.02496 |
| 5 Si -0.02251 -0.00557 -0.01222 0.02621 |
| 6 C 0.00907 0.00072 0.00493 0.01035 |
| 7 Si -0.00660 0.00277 -0.00606 0.00938 |
| 8 C 0.01651 -0.00461 -0.03083 0.03527 |
| 9 Si -0.01354 0.00359 -0.01109 0.01786 |
| 10 C 0.00021 0.02331 0.01316 0.02677 |
| 11 Al 0.01694 -0.01710 0.01984 0.03119 |
| 12 C 0.01344 0.02854 -0.03624 0.04805 |
| 13 Si 0.01381 -0.00489 -0.02246 0.02681 |
| 14 C 0.02090 0.00871 0.00638 0.02353 |
| 15 Si 0.00267 -0.04133 -0.01091 0.04283 |
| 16 C -0.00088 0.00158 -0.00212 0.00279 |
| 17 Si 0.00347 0.00356 0.01058 0.01169 |
| 18 C 0.00888 0.00899 0.01360 0.01857 |
| 19 Si -0.00601 -0.02423 -0.00375 0.02524 |
| 20 C -0.00210 0.02238 0.00261 0.02263 |
| 21 Si -0.00760 -0.02390 -0.00769 0.02624 |
| 22 C -0.00250 0.01084 -0.00823 0.01384 |
| 23 Si -0.01414 -0.01979 -0.00565 0.02497 |
+-----+
| Net force -0.01085 -0.00279 -0.07512 |
+-----+
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# Item: 0
# File: G:/SiC-Al-Ga/Tot_EN-STRESS-Forces-LSDA-SiCNT-(6.0)-1Al(Si).hdf5
# Title: Tot_EN-STRESS-Forces-LSDA-SiCNT-(6.0)-1Al(Si).hdf5 - Stress_0
# Type: Stress
+-----+
| Stress Report |
+-----+
| [[ 2.95507913e-04 4.45061659e-05 -7.06267193e-05] |
| [ 4.45061659e-05 -2.12051553e-04 -1.34155695e-05] |
| [-7.06267193e-05 -1.34155695e-05 -2.00724237e-04]] eV/Ang**3 |
+-----+
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Results for forces and stress in SWSiCNT with Ga-doped at Si site

```
# Item: 0
# File: G:/SiC-Al-Ga/Stress-Forces-LSDA-SiCNT-(6.0)-1Ga(Si).hdf5
# Title: Stress-Forces-LSDA-SiCNT-(6.0)-1Ga(Si).hdf5 - Forces_0
# Type: Forces
+-----+
| Forces Report |
+-----+
| Index Element Force (eV/Ang) |
| x y z magnitude |
+-----+
| 0 Si 0.04302 0.00000 -0.10210 0.11079 |
| 1 C 0.01397 -0.02358 0.09953 0.10324 |
| 2 C 0.02914 -0.00000 0.05649 0.06357 |
| 3 Si -0.07007 0.03608 -0.08614 0.11675 |
| 4 C 0.11739 0.01718 0.05622 0.13128 |
| 5 Si 0.00869 0.01943 -0.02093 0.02986 |
| 6 C 0.12844 -0.02183 0.06653 0.14628 |
| 7 Si -0.02600 -0.06826 -0.26683 0.27665 |
| 8 C 0.04190 0.02789 -0.25390 0.25884 |
| 9 Si -0.25450 0.03672 0.06716 0.26576 |
| 10 C 0.34818 0.46712 0.14581 0.60058 |
| 11 Ga -0.06505 -0.00000 -0.84776 0.85025 |
| 12 C 0.04190 -0.02788 -0.25390 0.25884 |
| 13 Si -0.47513 -1.10965 0.75547 1.42401 |
| 14 C 0.37835 0.00000 -0.11407 0.39517 |
| 15 Si -0.02600 0.06826 -0.26683 0.27665 |
| 16 C 0.11739 -0.01718 0.05621 0.13128 |
| 17 Si -0.47512 1.10965 0.75547 1.42401 |
| 18 C 0.34818 -0.46712 0.14581 0.60058 |
| 19 Si -0.07007 -0.03608 -0.08614 0.11675 |
| 20 C 0.01397 0.02358 0.09953 0.10324 |
| 21 Si -0.25450 -0.03672 0.06716 0.26576 |
| 22 C 0.12844 0.02183 0.06653 0.14628 |
| 23 Si 0.00869 -0.01943 -0.02093 0.02986 |
+-----+
| Net force 0.05120 0.00000 0.11839 |
+-----+

# Item: 0
# File: G:/SiC-Al-Ga/Stress-Forces-LSDA-SiCNT-(6.0)-1Ga(Si).hdf5
# Title: Stress-Forces-LSDA-SiCNT-(6.0)-1Ga(Si).hdf5 - Stress_0
# Type: Stress
+-----+
| Stress Report |
+-----+
| [[-0.00064378 0. -0.00078826] |
| [ 0. 0.00067598 0. ] |
| [-0.00078826 0. 0.00115212]] eV/Ang**3 |
+-----+
```

Results for forces and stress in SWSiCNT with Al-doped at C site

```
# Item: 0
# File: G:/SiC-Al-Ga/Al-Ga(C)-SiCNT/LSDA+U-SiCNT-(6.0)-1Al(1C).hdf5
# Title: LSDA+U-SiCNT-(6.0)-1Al(1C).hdf5 - Forces_0
# Type: Forces
+-----+
| Forces Report |
+-----+
| Index Element Force (eV/Ang) |
| x y z magnitude |
+-----+
| 0 Si 0.03055 0.00000 -0.02523 0.03962 |
| 1 C 0.02476 -0.00073 0.00443 0.02517 |
| 2 C 0.01822 -0.00000 0.00647 0.01933 |
| 3 Si -0.01133 -0.01064 -0.01820 0.02393 |
| 4 C 0.02210 -0.03361 0.01085 0.04166 |
| 5 Si 0.01850 0.00095 -0.00852 0.02039 |
| 6 C 0.01342 0.00175 -0.00416 0.01416 |
| 7 Si -0.02632 -0.04011 -0.01147 0.04932 |
| 8 C -0.01301 0.02702 -0.01581 0.03390 |
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| 9 Si -0.00829 -0.04593 -0.01572 0.04925 |
| 10 C 0.00028 -0.01886 0.00673 0.02003 |
| 11 Si -0.04692 0.00000 0.00090 0.04693 |
| 12 C -0.01301 -0.02702 -0.01581 0.03390 |
| 13 Si -0.01264 0.00596 0.00306 0.01430 |
| 14 Al -0.00299 -0.00000 -0.01007 0.01050 |
| 15 Si -0.02632 0.04011 -0.01147 0.04932 |
| 16 C 0.02210 0.03361 0.01085 0.04166 |
| 17 Si -0.01264 -0.00596 0.00306 0.01430 |
| 18 C 0.00028 0.01886 0.00673 0.02003 |
| 19 Si -0.01133 0.01064 -0.01820 0.02393 |
| 20 C 0.02476 0.00073 0.00443 0.02517 |
| 21 Si -0.00829 0.04593 -0.01572 0.04925 |
| 22 C 0.01342 -0.00175 -0.00416 0.01416 |
| 23 Si 0.01850 -0.00095 -0.00852 0.02039 |
+-----+
| Net force 0.01384 0.00000 -0.12554 |
+-----+

# Item: 0
# File: G:/SiC-Al-Ga/Al-Ga(C)-SiCNT/LSDA+U-SiCNT-(6.0)-1Al(1C).hdf5
# Title: LSDA+U-SiCNT-(6.0)-1Al(1C).hdf5 - Stress_0
# Type: Stress
+-----+
| Stress Report |
+-----+
| [[-5.29082395e-04 0.00000000e+00 -5.48109094e-05] |
| [ 0.00000000e+00 5.35811049e-04 0.00000000e+00] |
| [-5.48109094e-05 0.00000000e+00 -2.70002231e-04]] eV/Ang**3 |
+-----+

```

Results for forces and stress in SWSiCNT with Ga-doped at C site

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# Item: 0
# File: G:/SiC-Al-Ga/Al-Ga(C)-SiCNT/Y-LSDA+U-SiCNT-(6.0)-1Ga(1C).hdf5
# Title: Y-LSDA+U-SiCNT-(6.0)-1Ga(1C).hdf5 - Forces_0
# Type: Forces
+-----+
| Forces Report |
+-----+
| Index Element Force (eV/Ang) |
| x y z magnitude |
+-----+
| 0 Si 0.02234 0.00000 -0.00350 0.02261 |
| 1 C 0.02192 0.01440 -0.01068 0.02832 |
| 2 C 0.03165 -0.00000 -0.01193 0.03382 |
| 3 Si 0.01660 -0.00547 -0.00735 0.01896 |
| 4 C -0.00349 -0.01000 -0.00531 0.01184 |
| 5 Si 0.01737 0.00039 -0.00485 0.01804 |
| 6 C -0.00533 -0.00252 -0.00860 0.01043 |
| 7 Si 0.00586 -0.01720 -0.01724 0.02505 |
| 8 C -0.02081 -0.00480 -0.02448 0.03248 |
| 9 Si 0.00704 -0.02017 -0.00402 0.02174 |
| 10 C 0.00233 -0.03845 0.00129 0.03854 |
| 11 Si -0.04089 -0.00000 0.00020 0.04089 |
| 12 C -0.02081 0.00480 -0.02448 0.03248 |
| 13 Si -0.01873 -0.00418 0.00770 0.02068 |
| 14 Ga -0.04187 -0.00000 0.01540 0.04461 |
| 15 Si 0.00586 0.01720 -0.01724 0.02505 |
| 16 C -0.00349 0.01000 -0.00531 0.01184 |
| 17 Si -0.01873 0.00418 0.00770 0.02068 |
| 18 C 0.00233 0.03845 0.00129 0.03854 |
| 19 Si 0.01660 0.00547 -0.00735 0.01896 |
| 20 C 0.02192 -0.01440 -0.01068 0.02832 |
| 21 Si 0.00704 0.02017 -0.00402 0.02174 |
| 22 C -0.00533 0.00252 -0.00860 0.01043 |
| 23 Si 0.01737 -0.00039 -0.00485 0.01804 |
+-----+
| Net force 0.01676 -0.00000 -0.14691 |
+-----+

```

```
# Item: 0
# File: G:/SiC-Al-Ga/Al-Ga(C)-SiCNT/Y-LSDA+U-SiCNT-(6.0)-1Ga(1C).hdf5
# Title: Y-LSDA+U-SiCNT-(6.0)-1Ga(1C).hdf5 - Stress_0
# Type: Stress
+-----+
| Stress Report |
+-----+
| [[-6.23089459e-04 0.00000000e+00 -1.15914867e-05] |
| [ 0.00000000e+00 3.78149969e-04 0.00000000e+00] |
| [-1.15914867e-05 0.00000000e+00 -2.70356512e-04]] eV/Ang**3 |
+-----+
```