# Supplementary Information

## Strain- and chirality-engineered tunability of electronic and thermoelectric properties in SiC nanotubes: insights from first-principles calculations

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**Optimized crystal structure of (10,0) SiCNT (CIF format)**

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1


_chemical_name_common                  'nanotube'
_cell_length_a                         13.246300
_cell_length_b                         13.246300
_cell_length_c                         5.375500
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      120.000000
_cell_volume                           816.843149
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
```

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.0 | 0.873700 | 0.500000 | 0.333000 | Uiso | ? | C |
| Si | 1.0 | 0.873700 | 0.500000 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.922000 | 0.633300 | 0.833000 | Uiso | ? | C |
| Si | 1.0 | 0.922000 | 0.633300 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.929100 | 0.753600 | 0.333000 | Uiso | ? | C |
| Si | 1.0 | 0.929100 | 0.753600 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.894200 | 0.849100 | 0.833000 | Uiso | ? | C |
| Si | 1.0 | 0.894200 | 0.849100 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.820600 | 0.910400 | 0.333000 | Uiso | ? | C |
| Si | 1.0 | 0.820600 | 0.910400 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.715700 | 0.931500 | 0.833000 | Uiso | ? | C |
| Si | 1.0 | 0.715700 | 0.931500 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.589700 | 0.910400 | 0.333000 | Uiso | ? | C |
| Si | 1.0 | 0.589700 | 0.910400 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.454900 | 0.849100 | 0.833000 | Uiso | ? | C |
| Si | 1.0 | 0.454900 | 0.849100 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.324500 | 0.753600 | 0.333000 | Uiso | ? | C |
| Si | 1.0 | 0.324500 | 0.753600 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.211300 | 0.633300 | 0.833000 | Uiso | ? | C |
| Si | 1.0 | 0.211300 | 0.633300 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.126300 | 0.500000 | 0.333000 | Uiso | ? | C |
| Si | 1.0 | 0.126300 | 0.500000 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.078000 | 0.366700 | 0.833000 | Uiso | ? | C |
| Si | 1.0 | 0.078000 | 0.366700 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.070900 | 0.246400 | 0.333000 | Uiso | ? | C |
| Si | 1.0 | 0.070900 | 0.246400 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.105800 | 0.150900 | 0.833000 | Uiso | ? | C |
| Si | 1.0 | 0.105800 | 0.150900 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.179400 | 0.089600 | 0.333000 | Uiso | ? | C |
| Si | 1.0 | 0.179400 | 0.089600 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.284300 | 0.068500 | 0.833000 | Uiso | ? | C |

| | | | | | | |
|---|---|---|---|---|---|---|
| Si | 1.0 | 0.284300 | 0.068500 | 0.500000 | Uiso | ? Si |
| C | 1.0 | 0.410300 | 0.089600 | 0.333000 | Uiso | ? C |
| Si | 1.0 | 0.410300 | 0.089600 | 0.000000 | Uiso | ? Si |
| C | 1.0 | 0.545100 | 0.150900 | 0.833000 | Uiso | ? C |
| Si | 1.0 | 0.545100 | 0.150900 | 0.500000 | Uiso | ? Si |
| C | 1.0 | 0.675500 | 0.246400 | 0.333000 | Uiso | ? C |
| Si | 1.0 | 0.675500 | 0.246400 | 0.000000 | Uiso | ? Si |
| C | 1.0 | 0.788700 | 0.366700 | 0.833000 | Uiso | ? C |
| Si | 1.0 | 0.788700 | 0.366700 | 0.500000 | Uiso | ? Si |

**Optimized crystal structure of (11,0) SiCNT (CIF format)**

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'nanotube'
_cell_length_a                         14.230400
_cell_length_b                         14.230400
_cell_length_c                         5.374600
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      120.000000
_cell_volume                           942.564318
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
```

```
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   C        1.0   0.882400   0.500000   0.333100   Uiso  ? C
   Si       1.0   0.882400   0.500000   0.000000   Uiso  ? Si
   C        1.0   0.929100   0.624400   0.833100   Uiso  ? C
   Si       1.0   0.929100   0.624400   0.500000   Uiso  ? Si
   C        1.0   0.941100   0.738700   0.333100   Uiso  ? C
   Si       1.0   0.941100   0.738700   0.000000   Uiso  ? Si
   C        1.0   0.917300   0.833700   0.833100   Uiso  ? C
   Si       1.0   0.917300   0.833700   0.500000   Uiso  ? Si
   C        1.0   0.859700   0.901700   0.333100   Uiso  ? C
   Si       1.0   0.859700   0.901700   0.000000   Uiso  ? Si
   C        1.0   0.773000   0.937100   0.833100   Uiso  ? C
   Si       1.0   0.773000   0.937100   0.500000   Uiso  ? Si
   C        1.0   0.664100   0.937100   0.333100   Uiso  ? C
   Si       1.0   0.664100   0.937100   0.000000   Uiso  ? Si
   C        1.0   0.542000   0.901700   0.833100   Uiso  ? C
   Si       1.0   0.542000   0.901700   0.500000   Uiso  ? Si
   C        1.0   0.416400   0.833700   0.333100   Uiso  ? C
   Si       1.0   0.416400   0.833700   0.000000   Uiso  ? Si
   C        1.0   0.297700   0.738700   0.833100   Uiso  ? C
```

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Si | 1.0 | 0.297700 | 0.738700 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.195300 | 0.624400 | 0.333100 | Uiso | ? | C |
| Si | 1.0 | 0.195300 | 0.624400 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.117600 | 0.500000 | 0.833100 | Uiso | ? | C |
| Si | 1.0 | 0.117600 | 0.500000 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.070900 | 0.375600 | 0.333100 | Uiso | ? | C |
| Si | 1.0 | 0.070900 | 0.375600 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.058900 | 0.261300 | 0.833100 | Uiso | ? | C |
| Si | 1.0 | 0.058900 | 0.261300 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.082700 | 0.166300 | 0.333100 | Uiso | ? | C |
| Si | 1.0 | 0.082700 | 0.166300 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.140300 | 0.098300 | 0.833100 | Uiso | ? | C |
| Si | 1.0 | 0.140300 | 0.098300 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.227000 | 0.062900 | 0.333100 | Uiso | ? | C |
| Si | 1.0 | 0.227000 | 0.062900 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.335900 | 0.062900 | 0.833100 | Uiso | ? | C |
| Si | 1.0 | 0.335900 | 0.062900 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.458000 | 0.098300 | 0.333100 | Uiso | ? | C |
| Si | 1.0 | 0.458000 | 0.098300 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.583600 | 0.166300 | 0.833100 | Uiso | ? | C |
| Si | 1.0 | 0.583600 | 0.166300 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.702300 | 0.261300 | 0.333100 | Uiso | ? | C |
| Si | 1.0 | 0.702300 | 0.261300 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.804700 | 0.375600 | 0.833100 | Uiso | ? | C |
| Si | 1.0 | 0.804700 | 0.375600 | 0.500000 | Uiso | ? | Si |

**Optimized crystal structure of (6,0) SiCNT (CIF format)**

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1


_chemical_name_common                  'nanotube'
_cell_length_a                         9.319200
_cell_length_b                         9.319200
_cell_length_c                         5.385400
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      120.000000
_cell_volume                           405.047361
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
```

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.0 | 0.820400 | 0.500000 | 0.332400 | Uiso | ? | C |
| Si | 1.0 | 0.820400 | 0.500000 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.870000 | 0.685000 | 0.832400 | Uiso | ? | C |
| Si | 1.0 | 0.870000 | 0.685000 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.820400 | 0.820400 | 0.332400 | Uiso | ? | C |
| Si | 1.0 | 0.820400 | 0.820400 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.685000 | 0.870000 | 0.832400 | Uiso | ? | C |
| Si | 1.0 | 0.685000 | 0.870000 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.500000 | 0.820400 | 0.332400 | Uiso | ? | C |
| Si | 1.0 | 0.500000 | 0.820400 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.315000 | 0.685000 | 0.832400 | Uiso | ? | C |
| Si | 1.0 | 0.315000 | 0.685000 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.179600 | 0.500000 | 0.332400 | Uiso | ? | C |
| Si | 1.0 | 0.179600 | 0.500000 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.130000 | 0.315000 | 0.832400 | Uiso | ? | C |
| Si | 1.0 | 0.130000 | 0.315000 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.179600 | 0.179600 | 0.332400 | Uiso | ? | C |
| Si | 1.0 | 0.179600 | 0.179600 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.315000 | 0.130000 | 0.832400 | Uiso | ? | C |
| Si | 1.0 | 0.315000 | 0.130000 | 0.500000 | Uiso | ? | Si |
| C | 1.0 | 0.500000 | 0.179600 | 0.332400 | Uiso | ? | C |
| Si | 1.0 | 0.500000 | 0.179600 | 0.000000 | Uiso | ? | Si |
| C | 1.0 | 0.685000 | 0.315000 | 0.832400 | Uiso | ? | C |
| Si | 1.0 | 0.685000 | 0.315000 | 0.500000 | Uiso | ? | Si |

## Optimized crystal structure of (6,6) SiCNT (CIF format)

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1
```

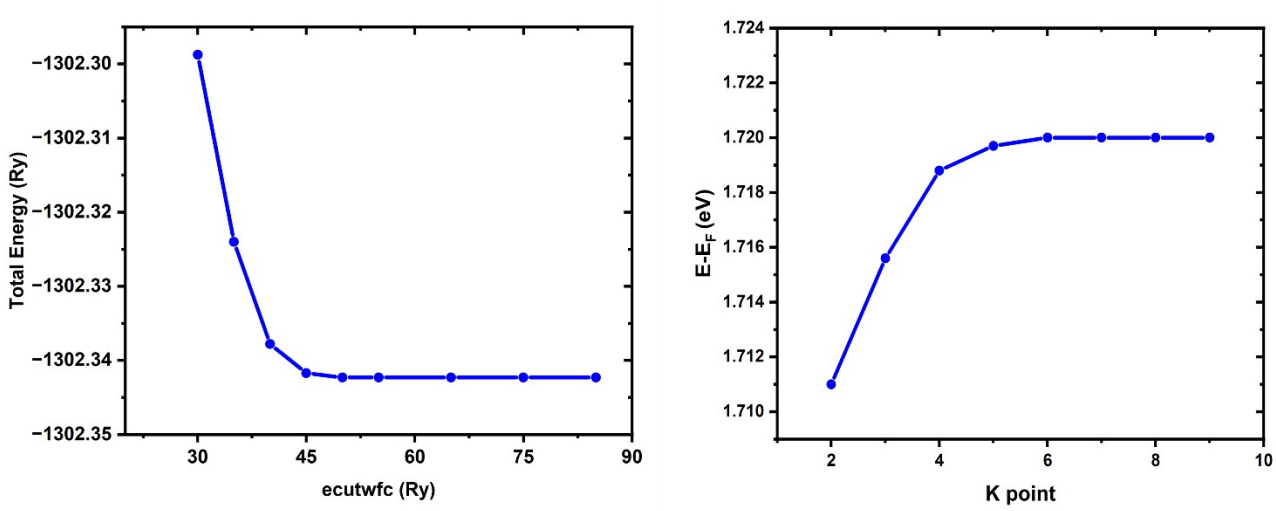
```
_chemical_name_common                  'nanotube'
_cell_length_a                         13.639000
_cell_length_b                         13.639000
_cell_length_c                         3.101300
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      120.000000
_cell_volume                           499.619598
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   Si         1.0     0.877300     0.500000     0.000000     Uiso  ? Si
   C          1.0     0.929100     0.649200     0.000000     Uiso  ? C
   Si         1.0     0.935700     0.717800     0.500000     Uiso  ? Si
   C          1.0     0.909300     0.833900     0.500000     Uiso  ? C
   Si         1.0     0.877300     0.877300     0.000000     Uiso  ? Si
   C          1.0     0.779900     0.929100     0.000000     Uiso  ? C
```

| | | | | | | |
|---|---|---|---|---|---|---|
| Si | 1.0 | 0.717800 | 0.935700 | 0.500000 | Uiso | ? Si |
| C | 1.0 | 0.575400 | 0.909300 | 0.500000 | Uiso | ? C |
| Si | 1.0 | 0.500000 | 0.877300 | 0.000000 | Uiso | ? Si |
| C | 1.0 | 0.350800 | 0.779900 | 0.000000 | Uiso | ? C |
| Si | 1.0 | 0.282200 | 0.717800 | 0.500000 | Uiso | ? Si |
| C | 1.0 | 0.166100 | 0.575400 | 0.500000 | Uiso | ? C |
| Si | 1.0 | 0.122700 | 0.500000 | 0.000000 | Uiso | ? Si |
| C | 1.0 | 0.070900 | 0.350800 | 0.000000 | Uiso | ? C |
| Si | 1.0 | 0.064300 | 0.282200 | 0.500000 | Uiso | ? Si |
| C | 1.0 | 0.090700 | 0.166100 | 0.500000 | Uiso | ? C |
| Si | 1.0 | 0.122700 | 0.122700 | 0.000000 | Uiso | ? Si |
| C | 1.0 | 0.220100 | 0.070900 | 0.000000 | Uiso | ? C |
| Si | 1.0 | 0.282200 | 0.064300 | 0.500000 | Uiso | ? Si |
| C | 1.0 | 0.424600 | 0.090700 | 0.500000 | Uiso | ? C |
| Si | 1.0 | 0.500000 | 0.122700 | 0.000000 | Uiso | ? Si |
| C | 1.0 | 0.649200 | 0.220100 | 0.000000 | Uiso | ? C |
| Si | 1.0 | 0.717800 | 0.282200 | 0.500000 | Uiso | ? Si |
| C | 1.0 | 0.833900 | 0.424600 | 0.500000 | Uiso | ? C |

**Figure S1**




(a) Cuttoff energy convergence for (10,0) SiCNT (b) k-point convergence of the bandgap for (10,0) SiCNT

**Fig. S1.** (a) Cutoff energy convergence for (10,0) SiCNT (b) k- point convergence of the bandgap for (10,0) SiCNT

**Figure S2**

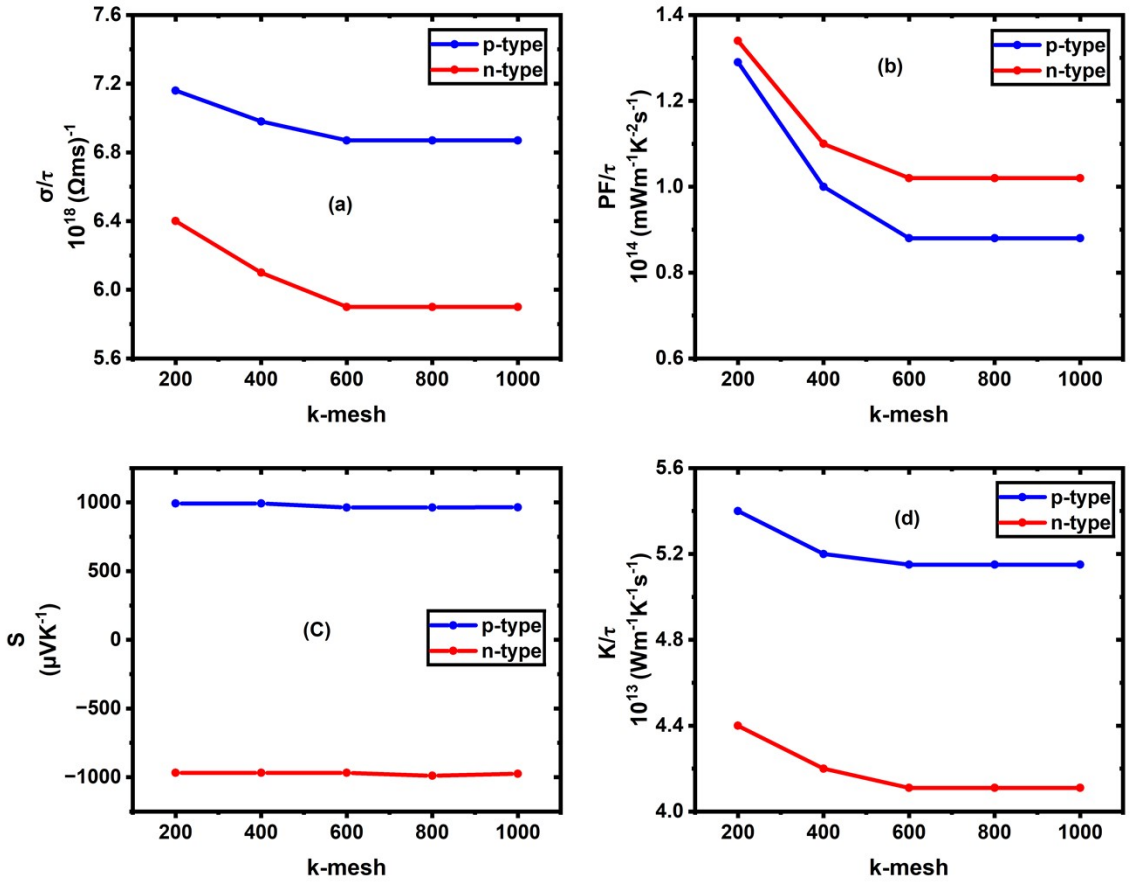



**Fig. S2.** k-mesh convergence of (a) electrical conductivity (σ/τ), (b) power factor (PF/τ), (c) Seebeck coefficient (S), and (d) electronic thermal conductivity (κ/τ) for the (6,0) SiCNT.

**Figure S3**

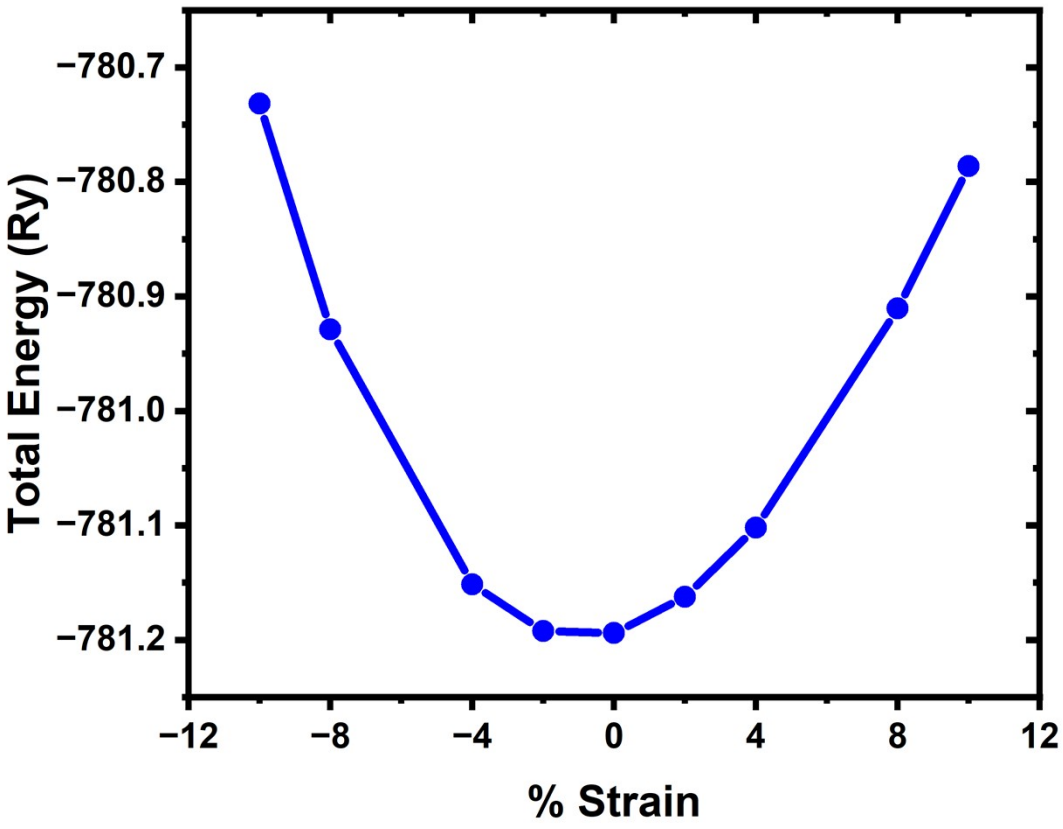



**Fig. S3.** Total energy as a function of applied uniaxial strain (−10% to +10%) for the (6,0) SiCNT

**Figure S4**

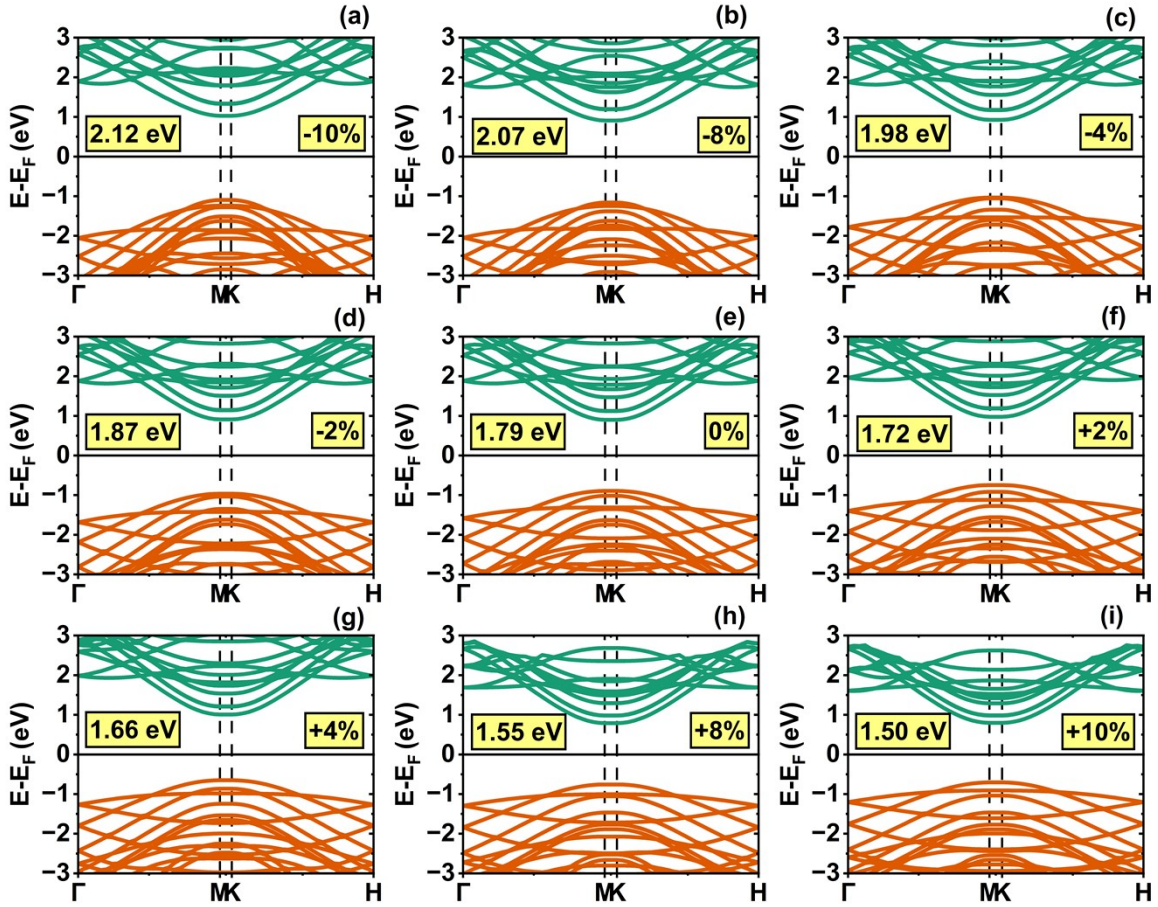



**Fig. S4.** Electronic band structures of the (11,0) single-walled SiCNT under uniaxial strain: (a) –10%, (b) –8%, (c) –4%, (d) –2%, (e) 0% (relaxed state), (f) +2%, (g) +4%, (h) +8%, and (i) +10%.

**Figure S5**

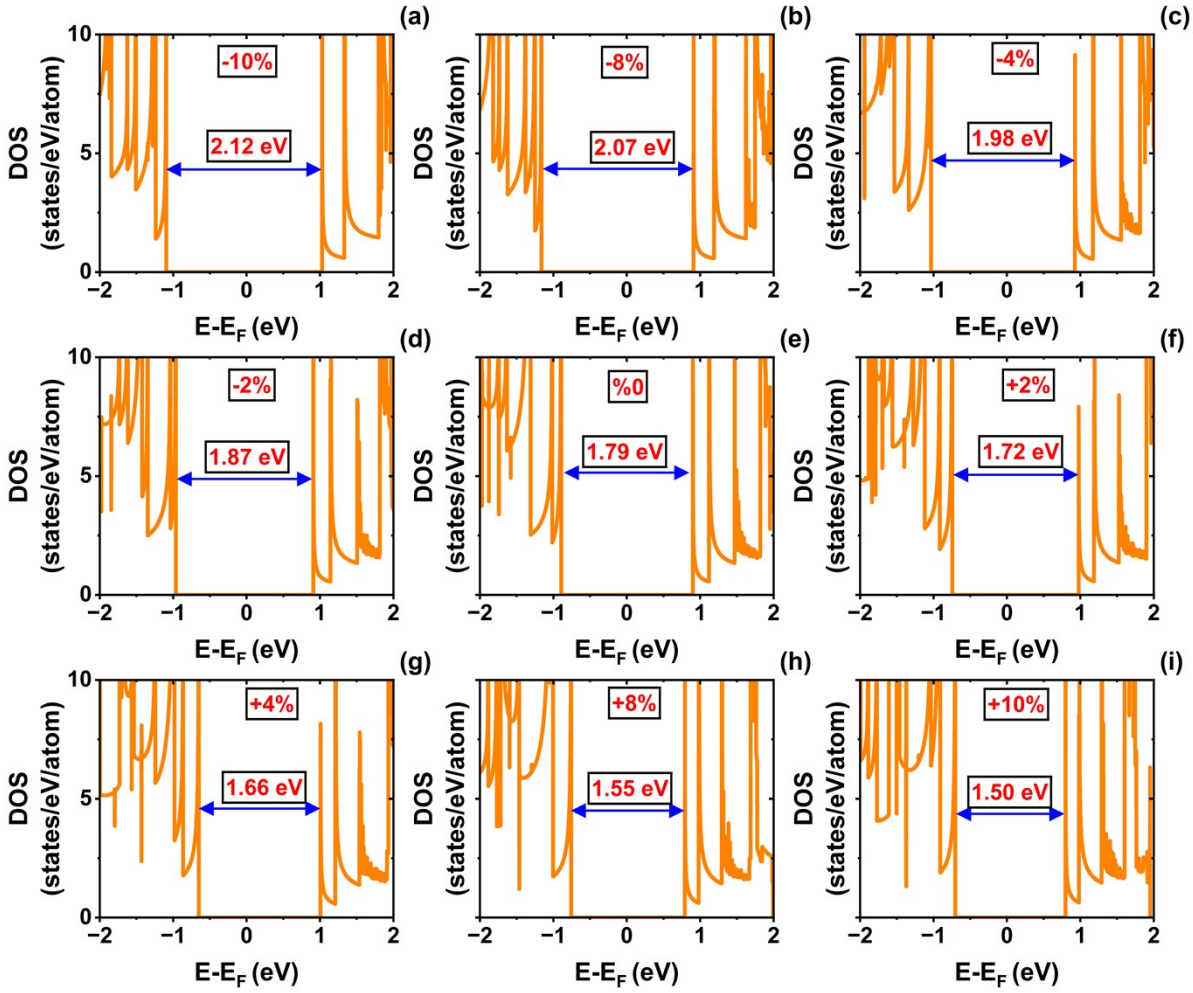



**Fig. S5.** Density of states (DOS) of the (11,0) single-walled SiCNT under uniaxial strain: (a) –10%, (b) –8%, (c) –4%, (d) –2%, (e) 0% (relaxed state), (f) +2%, (g) +4%, (h) +8%, and (i) +10%.

**Figure S6**

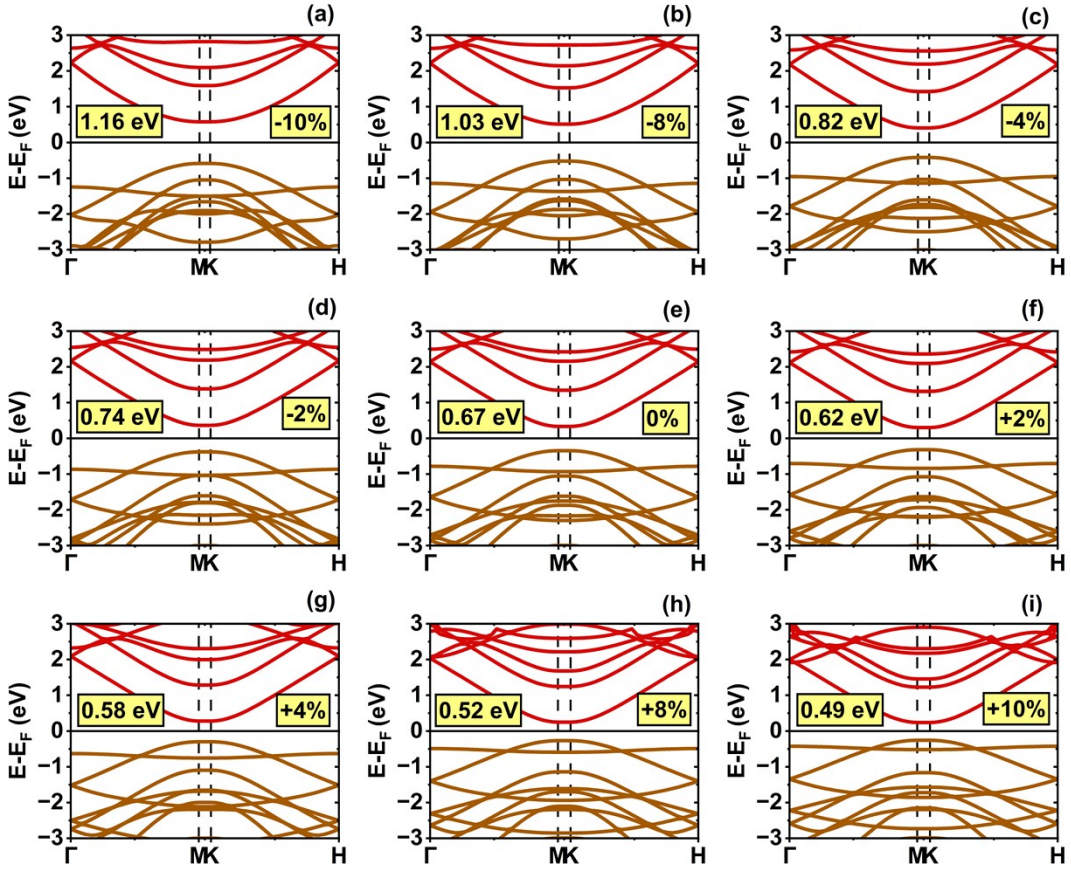



**Fig. S6.** Electronic band structures of the (6,0) single-walled SiCNT under uniaxial strain: (a) –10%, (b) –8%, (c) –4%, (d) –2%, (e) 0% (relaxed state), (f) +2%, (g) +4%, (h) +8%, and (i) +10%.

**Figure S7**

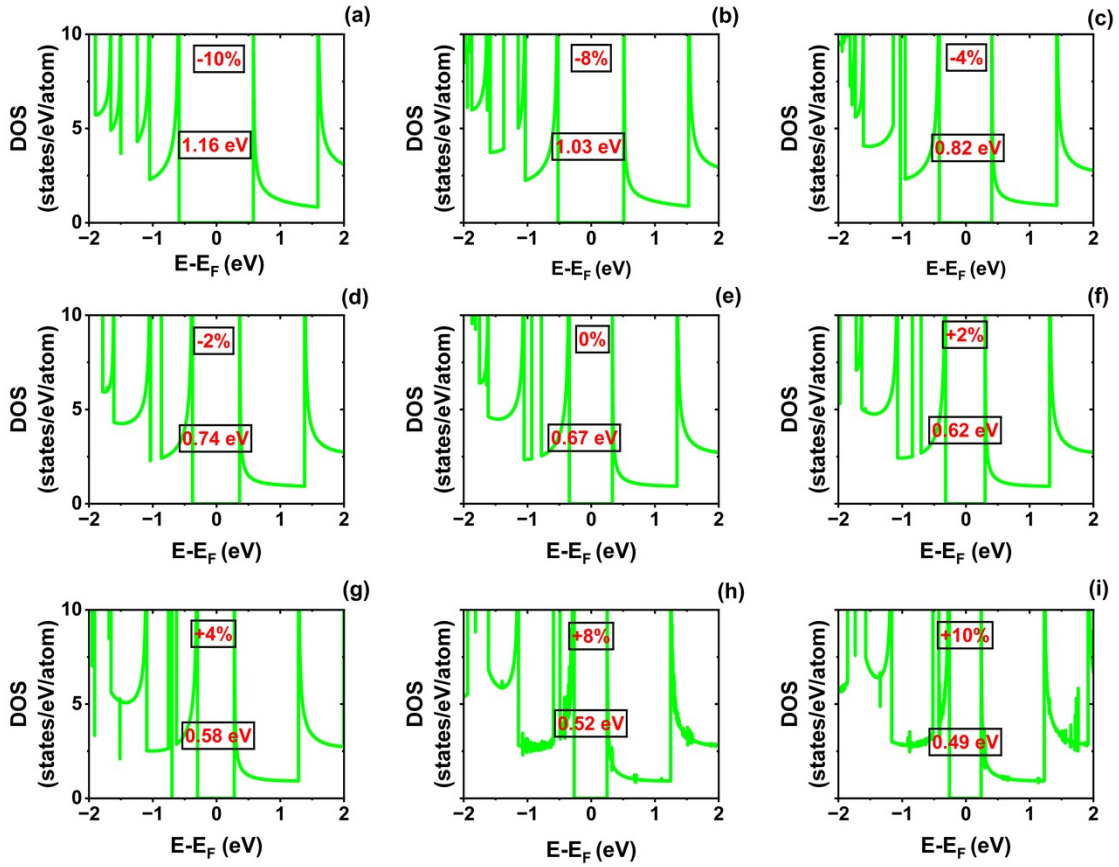



**Fig. S7.** Density of states (DOS) of the (6,0) single-walled SiCNT under uniaxial strain: (a) –10%, (b) –8%, (c) –4%, (d) –2%, (e) 0% (relaxed state), (f) +2%, (g) +4%, (h) +8%, and (i) +10%.

**Figure S8**

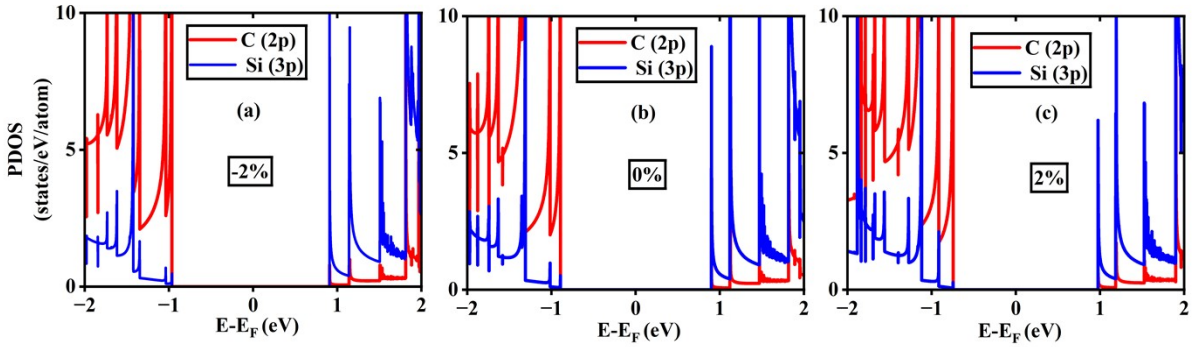



**Fig. S8.** Orbital-resolved PDOS of the (11,0) SiCNT under (a) −2%, (b) 0%, and (c) +2% strain, highlighting the contributions of C-2p and Si-3p states near the Fermi level.

**Table S1.** Comparison of bandgap values obtained using different exchange–correlation functionals and thermoelectric parameters of SiCNTs from literature and the present work

(A) Bandgap comparison using different theoretical methods for SWSiCNTs

| Nanotube | GGA (present work) | GGA (Literature) | LDA | HSE06(estimated)[1] |
|---|---|---|---|---|
| (6,0) | 0.67 eV | 0.68 eV[2] | 0.70 eV[3] | 1.70 eV |
| (10,0) | 1.72 eV | 1.76 eV[2] | 1.55 eV[4] | 2.55 eV |
| (11,0) | 1.79 eV | 1.87 eV[2] | ---- | ---- |
| (6,6) | 2.16 eV | 2.03 eV[5] | 1.78 eV[6] | 2.78 eV |

(B) Thermoelectric parameters from literature (SWCNTs)[7]

| Nanotube | Seebeck($\mu VK^{-1}$) | $\sigma/\tau$ ($\Omega^{-1} m^{-1} s^{-1}$) | PF/$\tau$ (mW $m^{-1} K^{-2} s^{-1}$) |
|---|---|---|---|
| (11,0) | 1579 (-3%) | $9.75 \times 10^{18}$ (-3%) | $1.55 \times 10^{14}$ (-9%) |
| (10,0) | 1580 (+3%) | $9.5 \times 10^{18}$ (-9%) | $1.44 \times 10^{14}$ (-3%) |
| (6,6) | 155 (-6%) | $2.03 \times 10^{19}$ (-9%) | $2.34 \times 10^{14}$ (-9%) |

(C) Thermoelectric parameters from the present work (SWSiCNTs)

| Nanotube | Seebeck($\mu VK^{-1}$) | $\sigma/\tau$ ($\Omega^{-1} m^{-1} s^{-1}$) | PF/$\tau$ (mW $m^{-1} K^{-2} s^{-1}$) |
|---|---|---|---|
| (11,0) | 1550.24 (-10% to +10%) | $1.72 \times 10^{19}$ (-10%) | $2.07 \times 10^{14}$ (-10%) |
| (10,0) | 1550.9 (0%) | $1.46 \times 10^{19}$ (-10%) | $1.36 \times 10^{14}$ (-0% to -2%) |
| (6,6) | 1550 (-10% to +10%) | $2.29 \times 10^{19}$ (-10%) | $1.95 \times 10^{14}$ (+10%) |

**References**


1 H. C. Hsueh, G. Y. Guo and S. G. Louie, Excitonic effects in the optical properties of SiC sheet and nanotubes, DOI:10.48550/ARXIV.1105.5531.

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