Supplementary Information

# Reducing Deformation of Single-walled Defective Silicon Carbide Nanotubes Under Charge Injection: A First Principles Study

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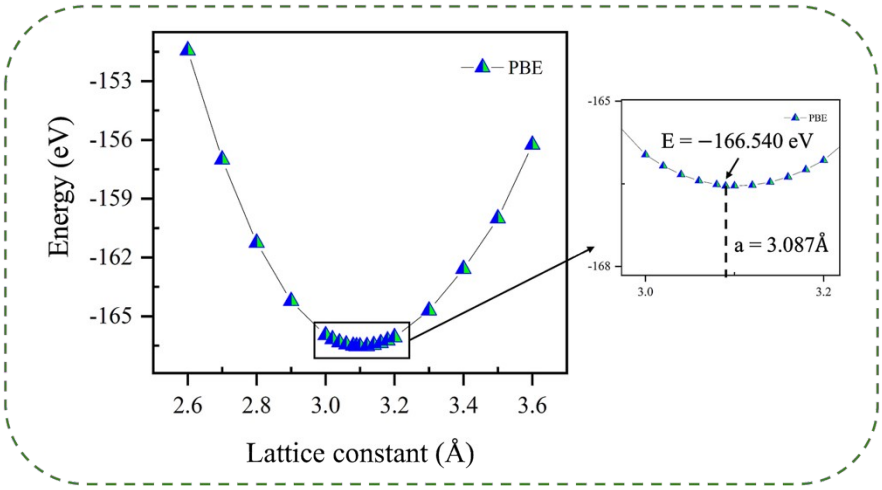



**Fig. S1**. Total energy of the (6,6) D-SiCNT as a function of applied strain along a-axis. The equilibrium lattice constant (a) and respective total energy are shown in the box.

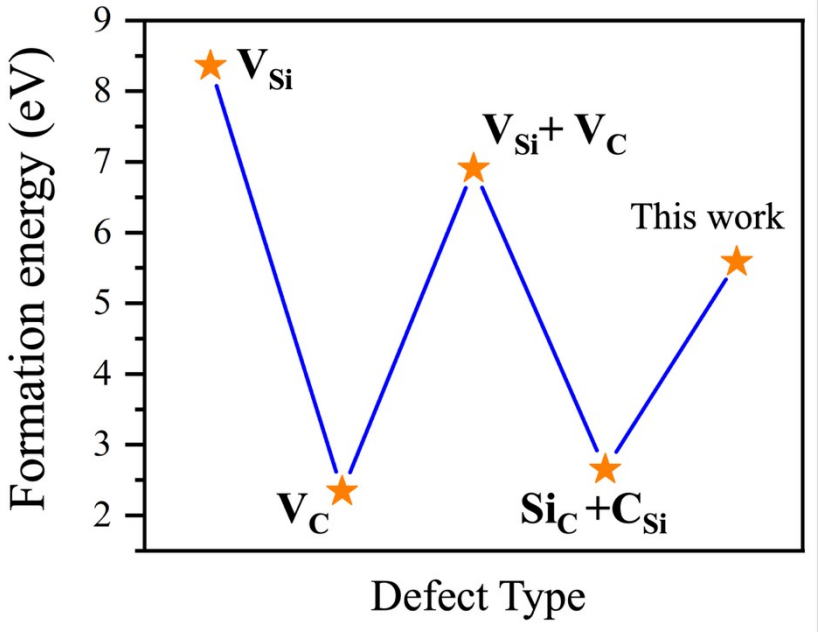
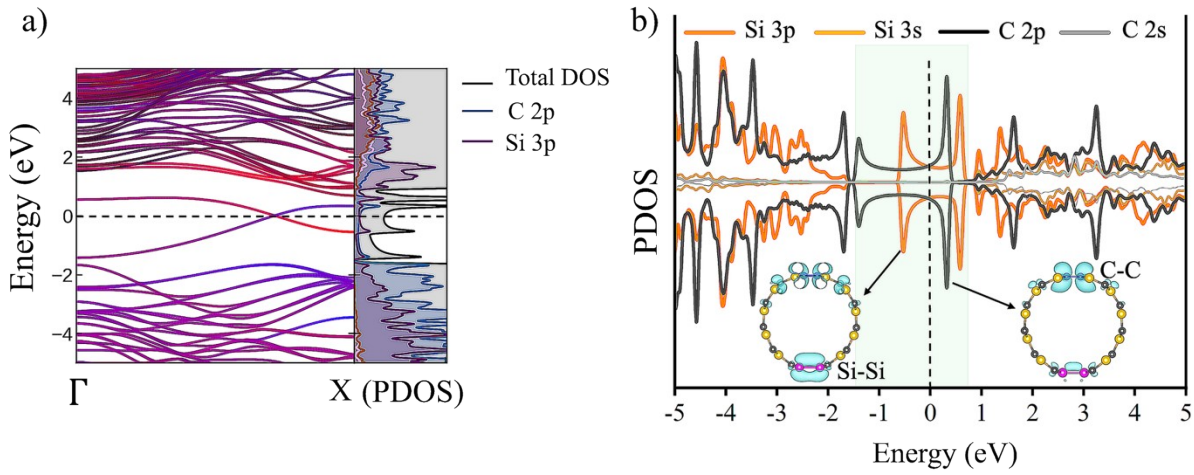



**Fig. S2.** Formation energy for various structural defects in (6,6) P-SiCNT.




**Fig, S3.** (a) Band structure with orbital-projected analysis for (6,6) D-SiCNT, highlighting the contributions from Si 3p and C 2p-orbitals. b) Partial density of states (PDOS) of the Si and C atoms forming the dimers on either side of the nanotube. The shaded energy region corresponds to the states used for the partial charge density (PARCHG) analysis. In the charge density plot, regions of charge accumulation are shown in cyan. Pink and blue sphere denote the Si and C dimers, respectively. The isosurface value $0.0003e^{-}/\text{Å}^3$ was used.

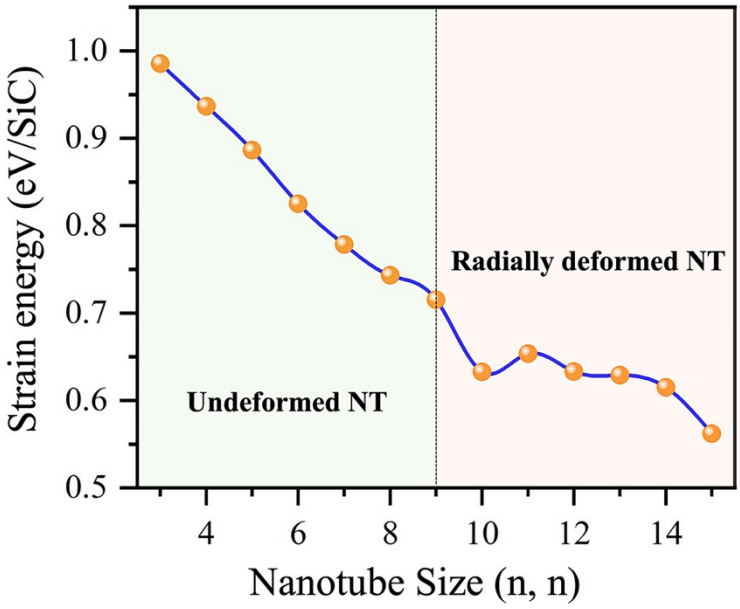



**Fig. S4.** Calculated strain energy as a function of D-SiCNTs for NTs ranging from (3,3) to (15,15).

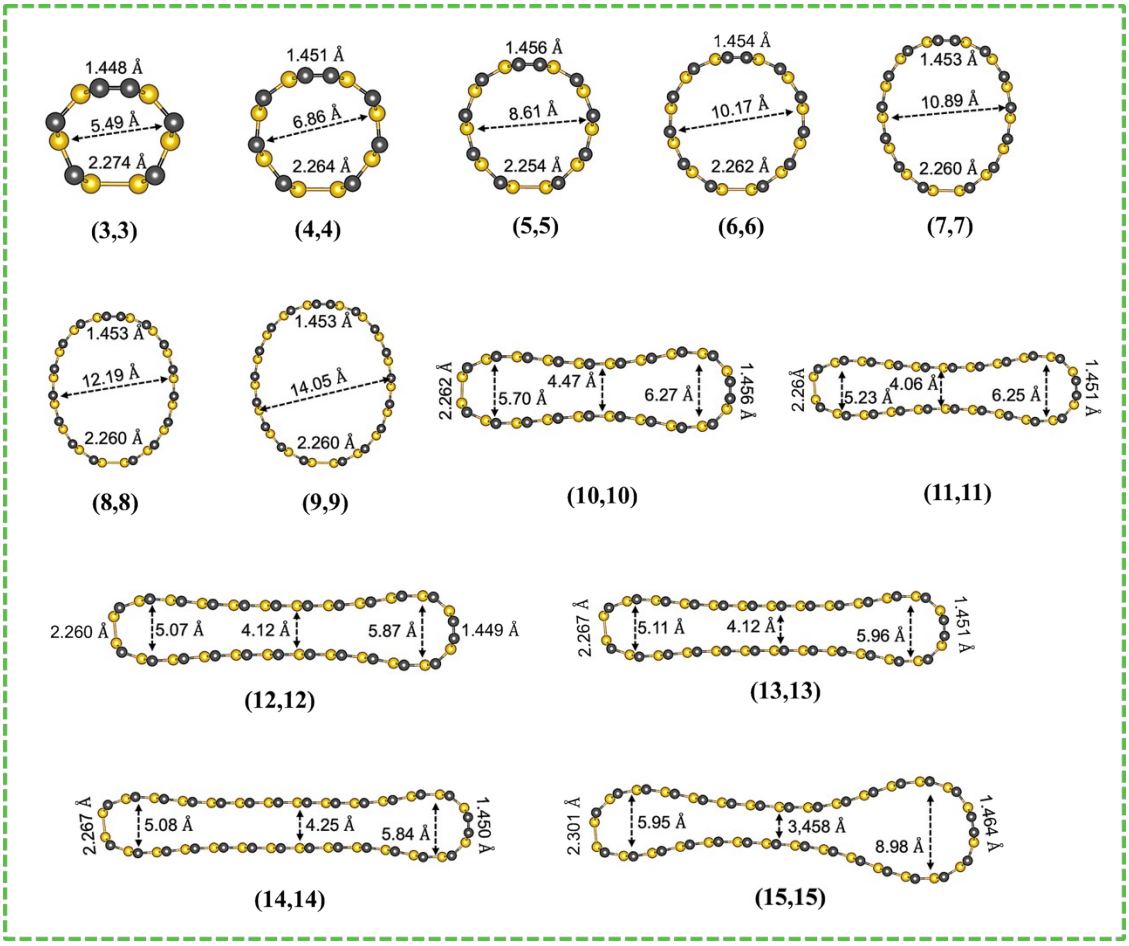



**Fig. S5.** Cross section view of the optimized D-SiCNTs structures ranging from (3,3), to (15,15), with annotated Si-Si and C-C bond lengths and nanotube diameters.

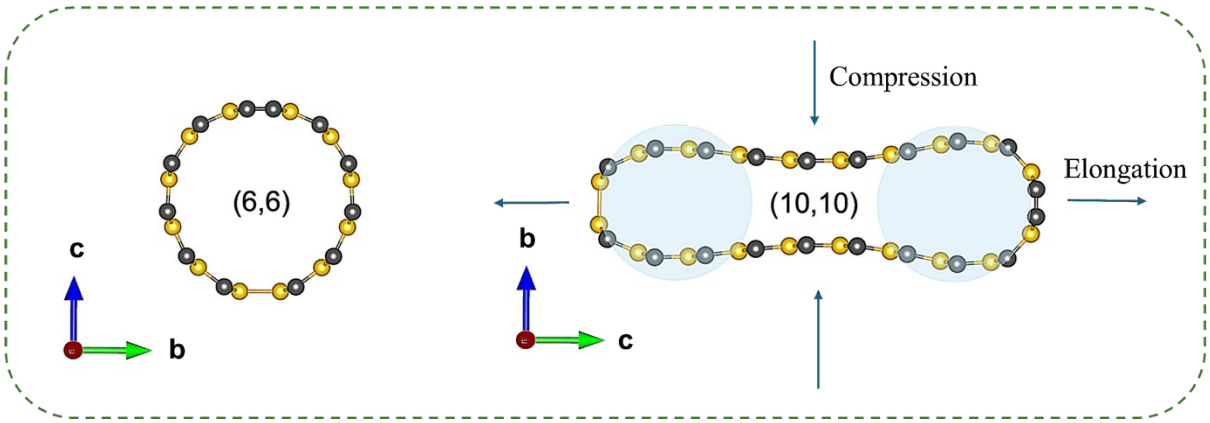



**Fig. S6.** Structure of the (6,6) (left) and (10,10) (right) D-SiCNTs, the (6,6) D-SiCNT is undeformed while the (10,10) D-SiCNT is distorted as it is contracted along the c-axis and elongated along the b-axis, resulting in a peanut-shaped configuration.

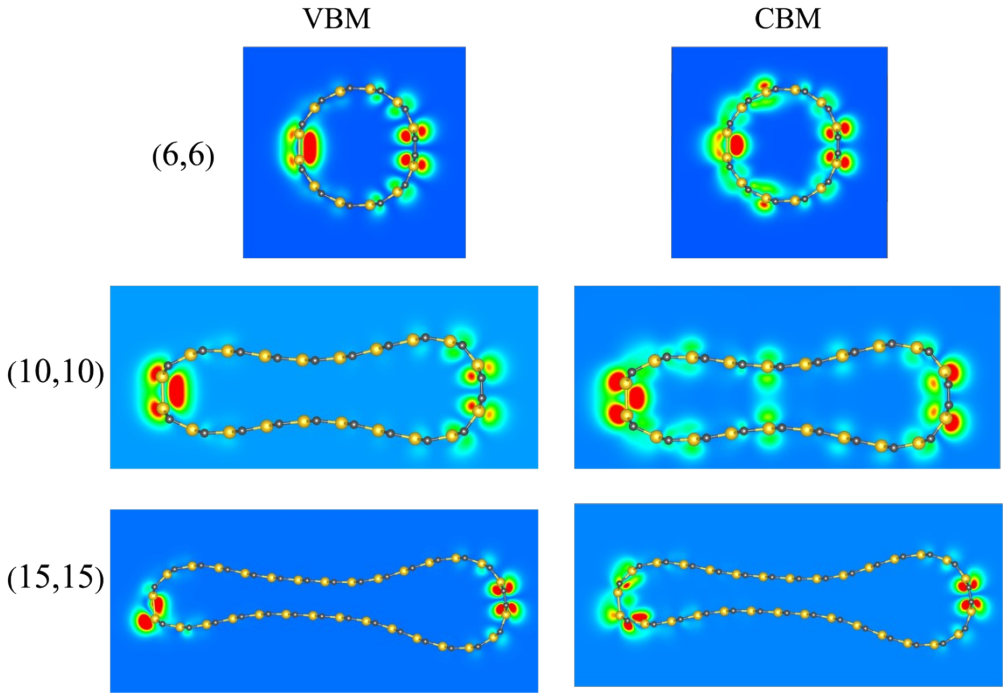



**Fig. S7.** Charge density distributions corresponding to the valence band maximum (VBM) and conduction band minimum (CBM) states for the undeformed (6,6) D-SiCNT and radially deformed (10,10) and (15,15) D-SiCNTs. Silicon and carbon atoms are represented by yellow and grey spheres, respectively. The red isosurface highlight regions of electron localization.

**Calculate the charge density for unit cell surface area:**

For the charge injection applying limit in our calculations is 0.15 $e^-$/atom. Considering this charge, we estimated the surface charge density as follows.

Surface area of (10,10) D-SiCNT of unit cell:

Diameter (D) =15.03 Å {for radially deformed D-SiCNT, average value will be taken}

Surface area (A) $= \pi \times D \times a$ {a is the lattice parameter of D-SiCNT}

$= \pi \times 15.03\ \text{Å} \times 3.09\ \text{Å}$

$= 1.462\ nm^2 = 1.46 \times 10^{-14}\ cm^2$

Surface charge density $= \dfrac{6\ e^-}{1.46 \times 10^{-14}\ cm^2}$ (Total charge injected per unit cell 6 $e^-$)

$= 4.1 \times 10^{14}\ e^-/cm^2$

Based on our study, this charge concentration per unit cell area corresponds to ~$10^{14}\ e^-/cm^2$, which falls within the range accessible via electrostatic gating or ionic liquid techniques, and other several methods. [1–5]

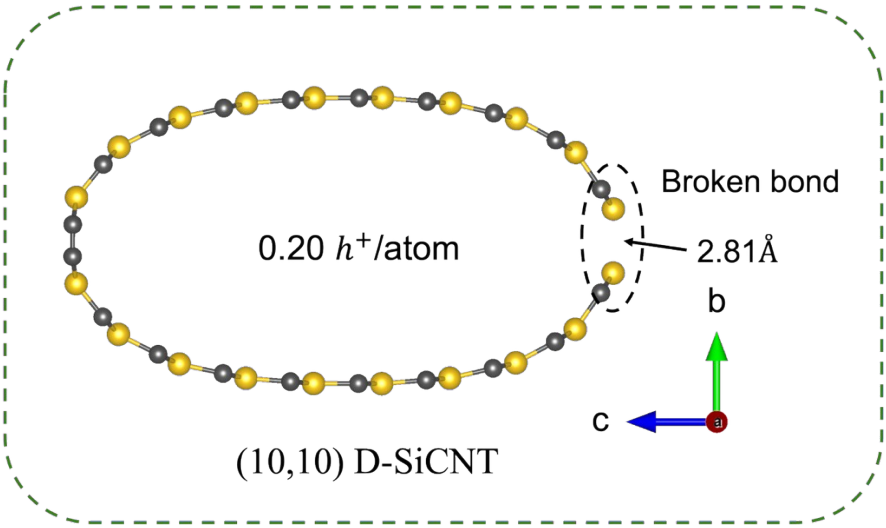



**Fig. S8.** Cross-section of the (10,10) D-SiCNT upon hole injection of +0.20 $h^+$/atom, that leads to it rupturing.

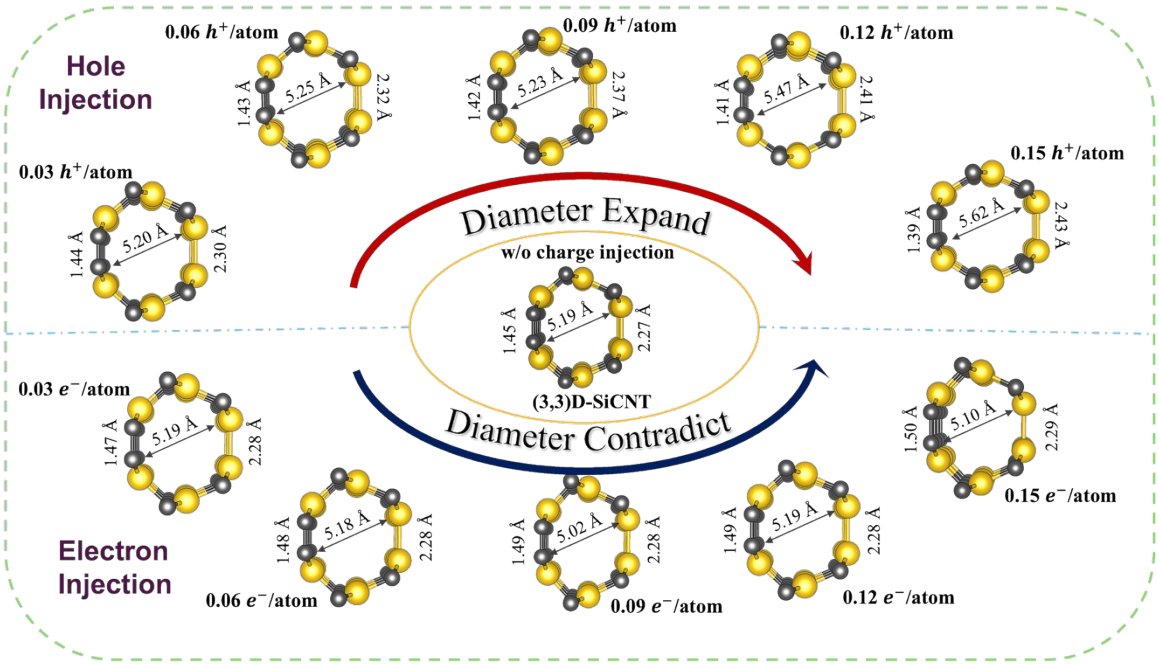



**Fig. S9.** Cross-sectional view of the (3,3) D-SiCNT (shown in the center). The top panel presents the optimized structures under hole injection, while the bottom panel shows the optimized structures after electron injection, each ranging from 0.03 to 0.15 $e^-$/atom.

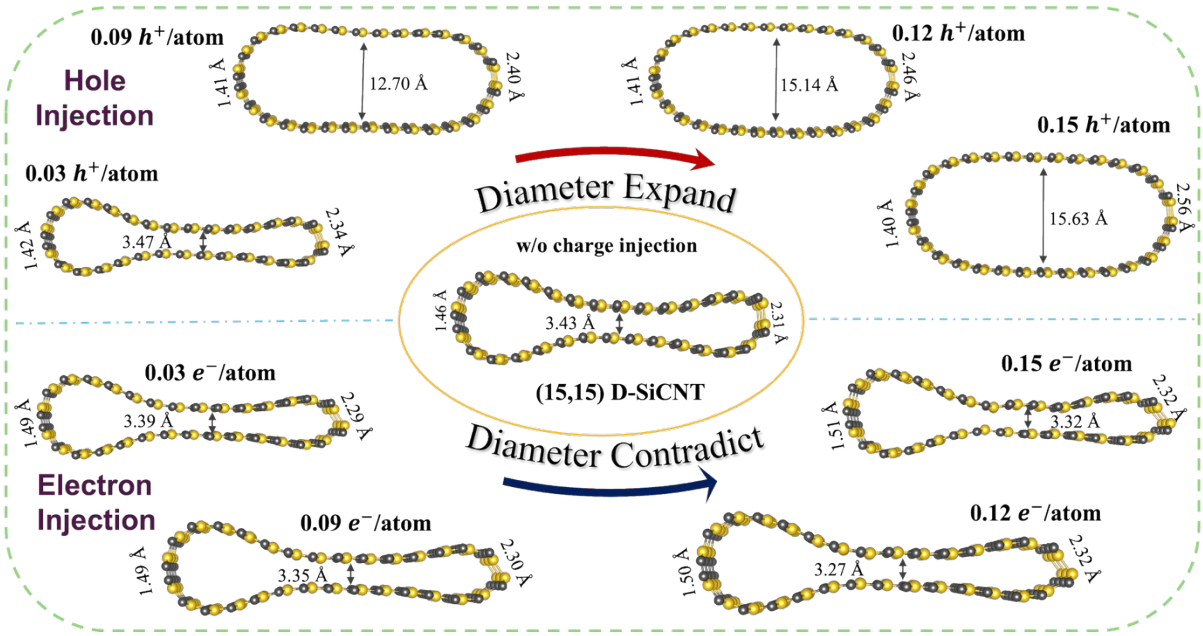


**Fig. S10.** Cross-sectional view of the radially deformed (15,15) D-SiCNT (shown in the center). The top panel presents the optimized structures under hole injection, while the bottom panel shows the optimized structures after electron injection, each ranging from 0.03 to 0.15 $e^-$/atom.

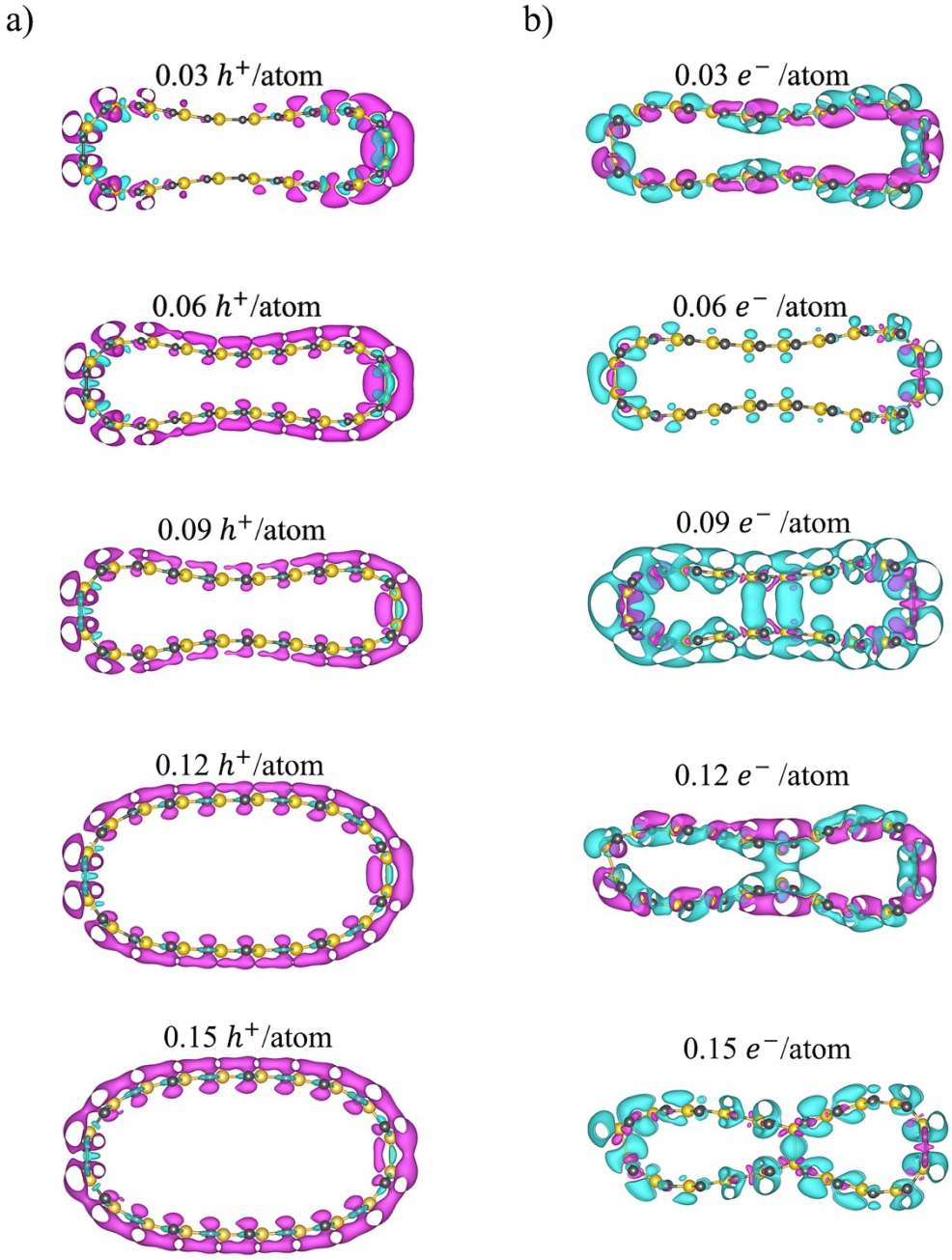



**Fig. S11.** Side view of the excess charge density distribution of the (10,10) D-SiCNT upon (a) charge injection and (b)electron injection ($e^-$/atom). The iso-surface value of 0.0003 e/Å$^3$ is used.

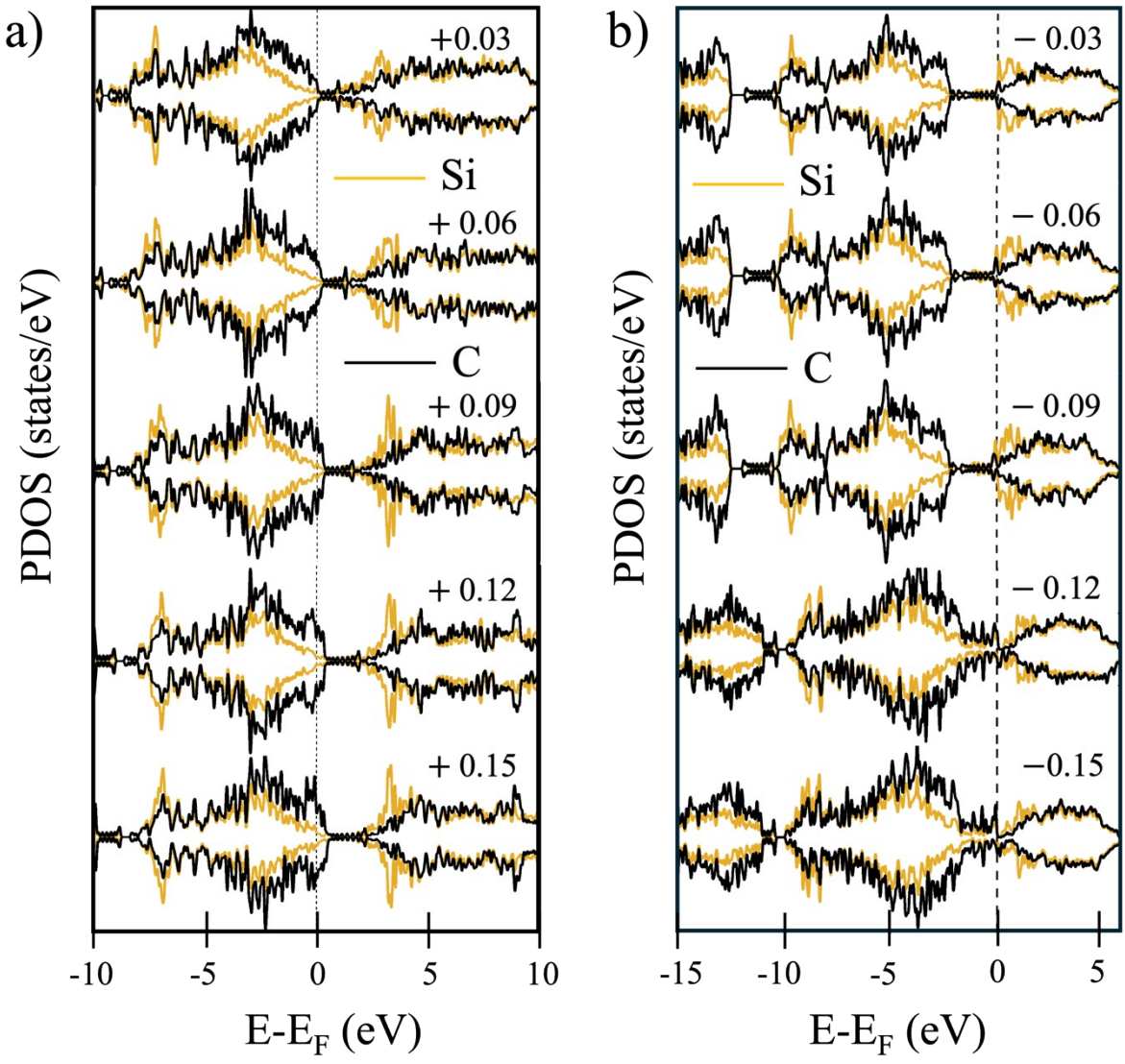



**Fig. S12.** Density of states of the (10,10) D-SiCNTs upon (a) hole injection (+0.03 to +0.15 $h^+$/atom) and (b) electron injection (-0.03 to -0.15 $e^-$/atom).

**Reference:**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3 J. T. Ye, Y. J. Zhang, R. Akashi, M. S. Bahramy, R. Arita and Y. Iwasa, *Science (1979)*, 2012, **338**, 1193–1196.

4 W. Shi, J. Ye, Y. Zhang, R. Suzuki, M. Yoshida, J. Miyazaki, N. Inoue, Y. Saito and Y. Iwasa, *Sci Rep*, 2015, **5**, 12534.

5 J. Ye, M. F. Craciun, M. Koshino, S. Russo, S. Inoue, H. Yuan, H. Shimotani, A. F. Morpurgo and Y. Iwasa, *Proceedings of the National Academy of Sciences*, 2011, **108**, 13002–13006.