

Electronic supplementary information

The transport properties of silicon and carbon nanotubes at the atomic scale: A first-principles study

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Content

1. The theoretical model with different buffer layers for armchair (3, 3) SiNTs.
2. Current-voltage, $I-V_b$, characteristic for **Model 1** and **Model 2**.
3. The relative energies of all systems in different Monkhorst-Pack grids and grid mesh cutoff.

1. The theoretical model with different Au atomic buffer layers, armchair (3, 3) SiNT is taken as an example. **Model 1** includes two and one atomic layers of Au atoms for the left and right of the molecule, and **Model 2** includes four and three atomic layers of Au atoms for the left and right of the molecule.

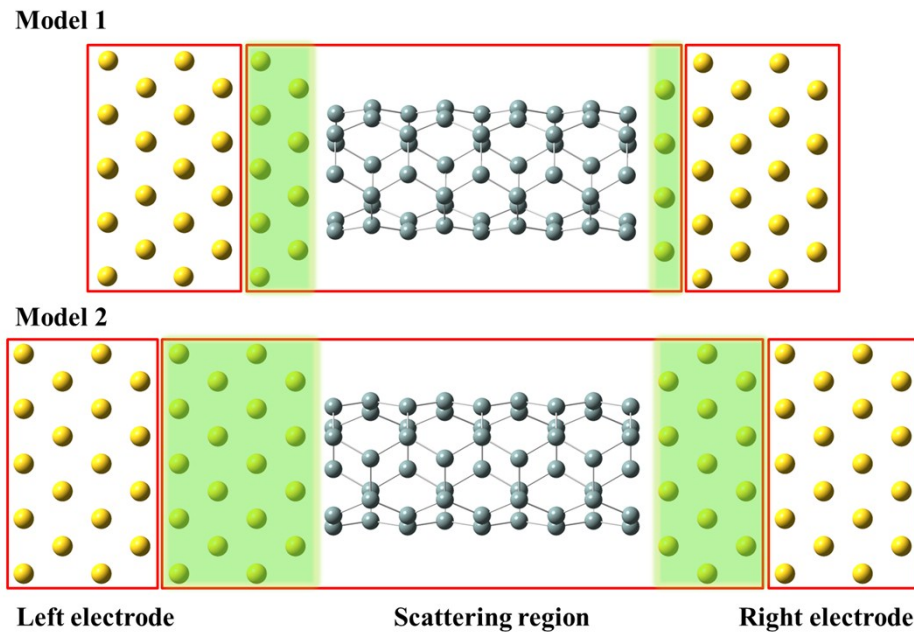


Fig. S1 The theoretical model with different buffer layers for armchair (3, 3) SiNTs.

2. The corresponding Current-voltage characteristic **Model 1** and **Model 2**, respectively.

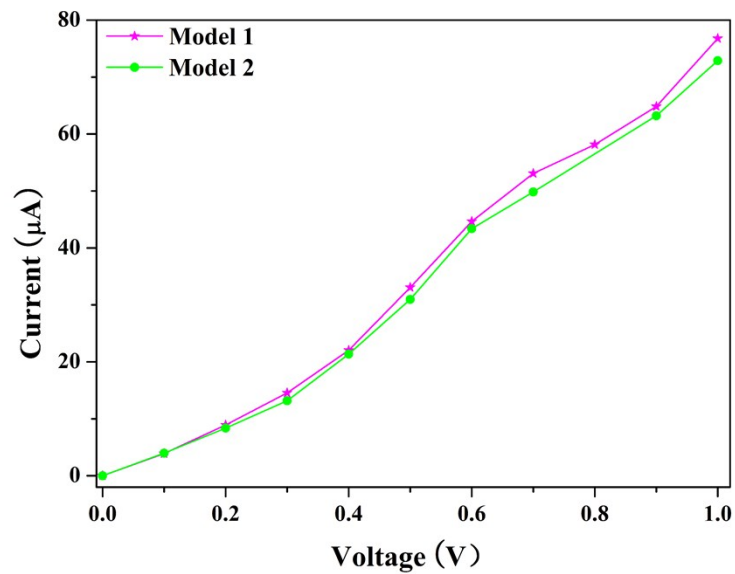


Fig. S2 Current-voltage, $I-V_b$, characteristic for **Model 1** and **Model 2**.

3. The Brillouin-zone sampling and the energy cutoff of the calculations are simulated at different values.

Table S1 The relative energies of all systems in different Monkorts-Pack grids and grid mesh cutoff.

Monkhorts-Pack grids	1×1×20			1×1×40	1×1×60
grid mesh cutoff	250 Ry	300 Ry	350 Ry	250 Ry	250 Ry
Si (3,3)	0	-1.4E-02	2.5E-03	1.5E-05	1.4E-05
Si (5, 0)	0	3.2 E-04	6.6 E-04	1E-06	1E-06
Si (6, 0)	0	-2.2E-03	8.2 E-04	-3E-05	-6.6E-05
Si (7, 0)	0	5.4E-04	1.2 E-03	-5E-05	-5.2E-05
C (3,3)	0	-3.1E-02	-3.3 E-02	-2.8E-03	-4.7E-03
C (5, 0)	0	-1.3E-02	-1.9 E-02	-9.6E-05	-9.3E-05
C (6, 0)	0	-2.2E-02	-2.9 E-02	2.5E-05	3.2E-05
C (7, 0)	0	-2.0E-02	-2.7 E-02	-1.3E-04	-1.0E-04