Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY MATERIALS

For

Chirality and Length-Dependent Electron Transmission of Fullerene-Capped Chiral Carbon Nanotubes Sandwiched in Gold Electrodes

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1. **Geometries of chiral (8, *m*) systems**

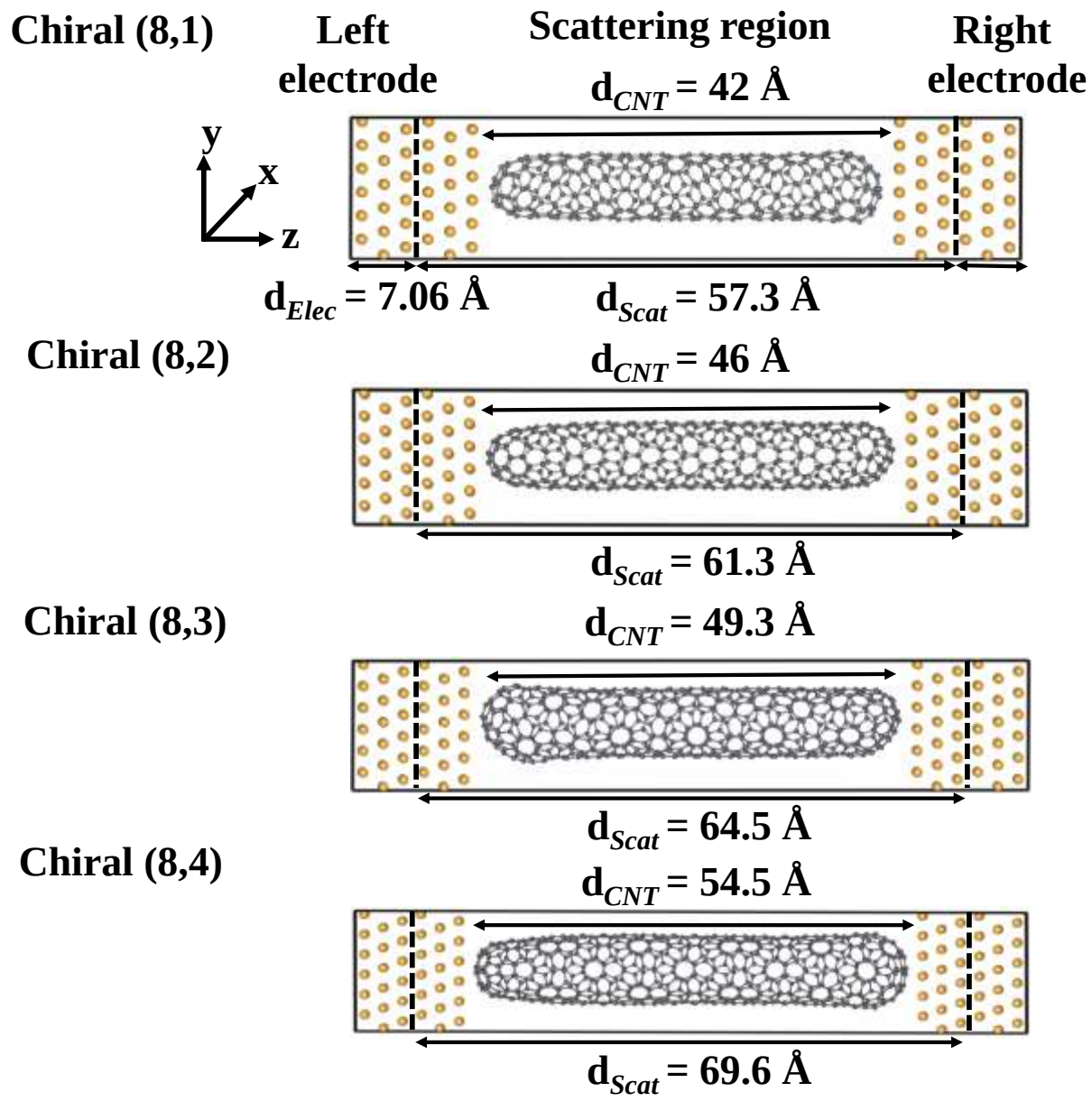

Figure S1. Device geometries (Au|CNT|Au) of Chiral (8,1), (8,2), (8,3), and (8,4) systems with similar length approximately 50 Å.

2. DOS of chiral (8, *m*)$_{S/L}$

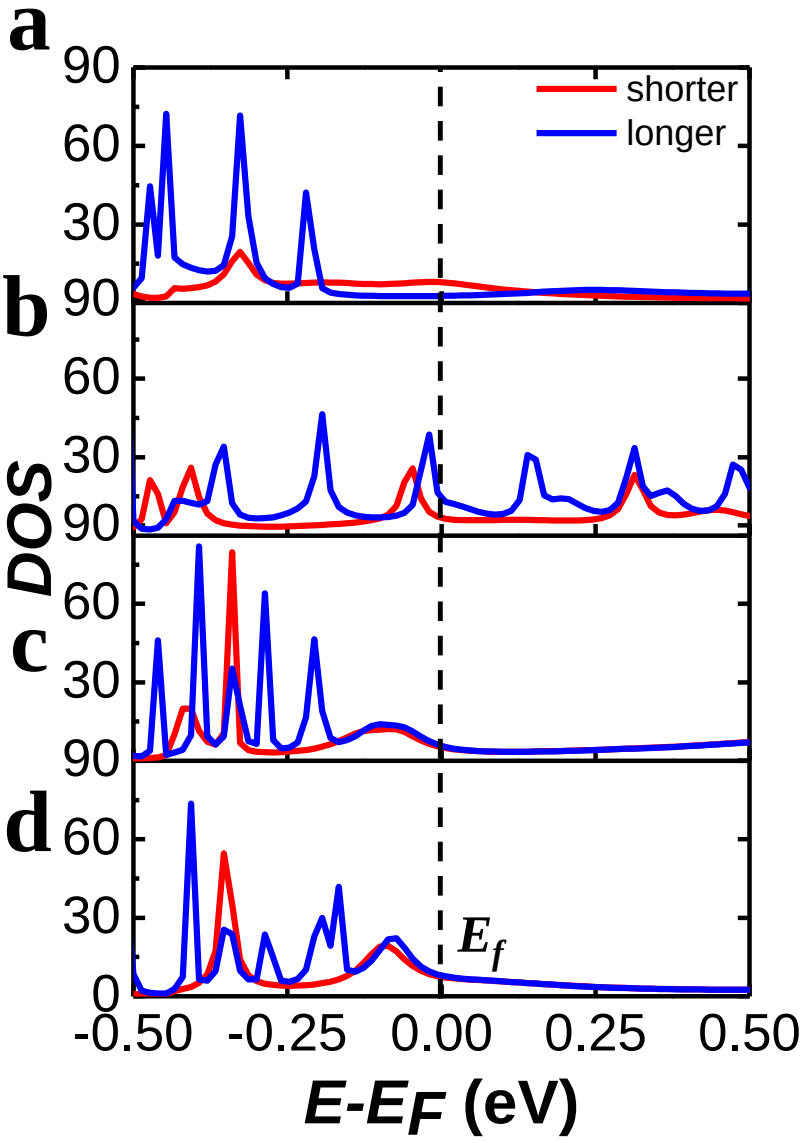

Figure S2. DOS spectra of chiral (8, 1)$_{S/L}$ (a), (8, 2)$_{S/L}$ (b), (8, 3)$_{S/L}$ (c), and (8, 4)$_{S/L}$ (d) at the zero-bias voltage. Red color shows shorter and blue color shows longer nanotube.

Figure S2 shows the density of states (DOS) of chiral (8, m)$_{S/L}$ CNTs. Figure S2a demonstrated that the DOS of chiral (8, 1) with shorter length had a small peak while longer length exhibited a bandgap near the

E_f. This observation confirms that the shorter nanotube has metallic properties and the longer nanotube has semiconducting features. The DOS of chiral (8, 2) (Figure S2b) shows prominent peaks near the E_f along both shorter and longer nanotubes which confirms that length variation did not significantly affect the electron transmission properties. The DOS of chiral (8, 3) and (8, 4) are shown in Figures S2c and S2d, respectively. For both shorter and longer nanotubes, a large bandgap was observed near the E_f. This bandgap denoted the semiconducting nature of the system.

3. Wavefunctions of (8, m)$_{S/L}$

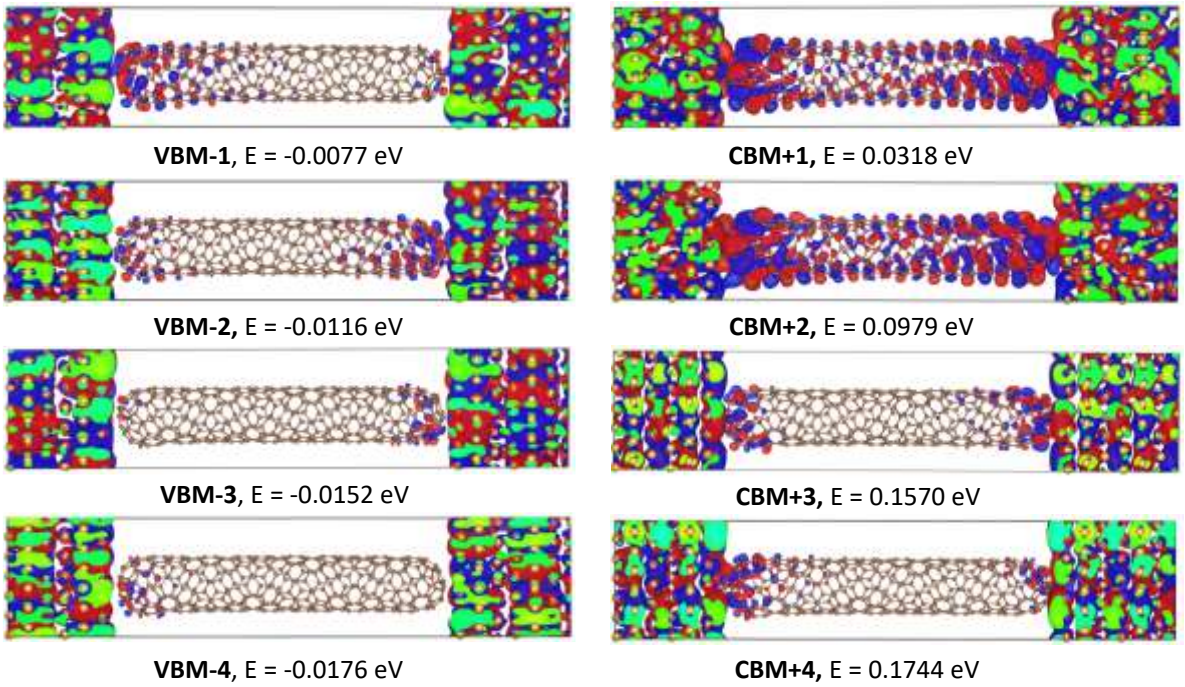

Figure S3. The wavefunction of Chiral (8, 1)$_S$. The isosurface value is 0.009 electrons/Å^3.

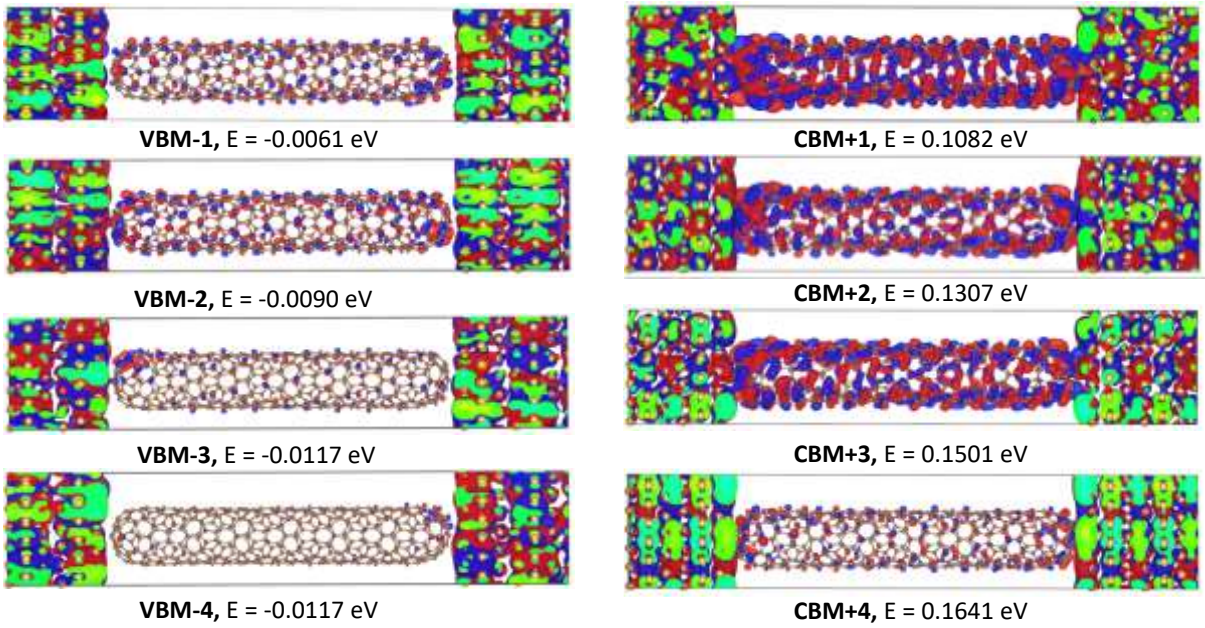

Figure S4. The wavefunctions of Chiral (8, 2)$_S$. The isosurface value is 0.009 electrons/Å^3.

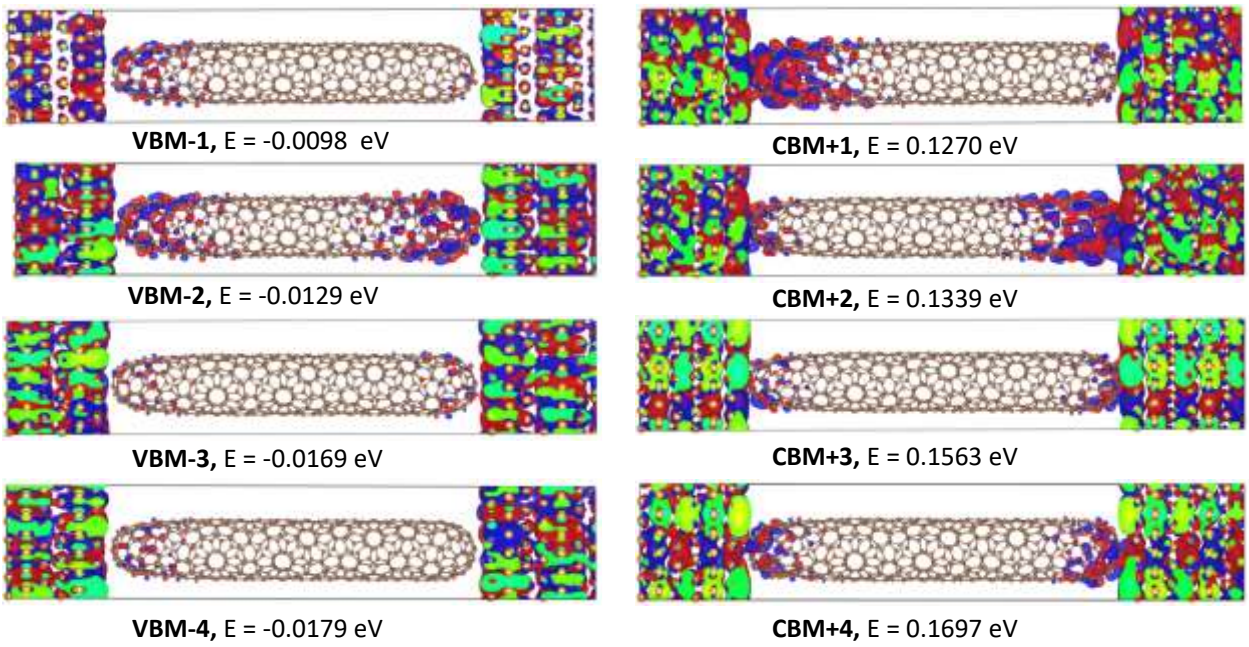

Figure S5: The wavefunctions of Chiral $(8, 3)_S$. The isosurface value is 0.009 electrons/Å^3.

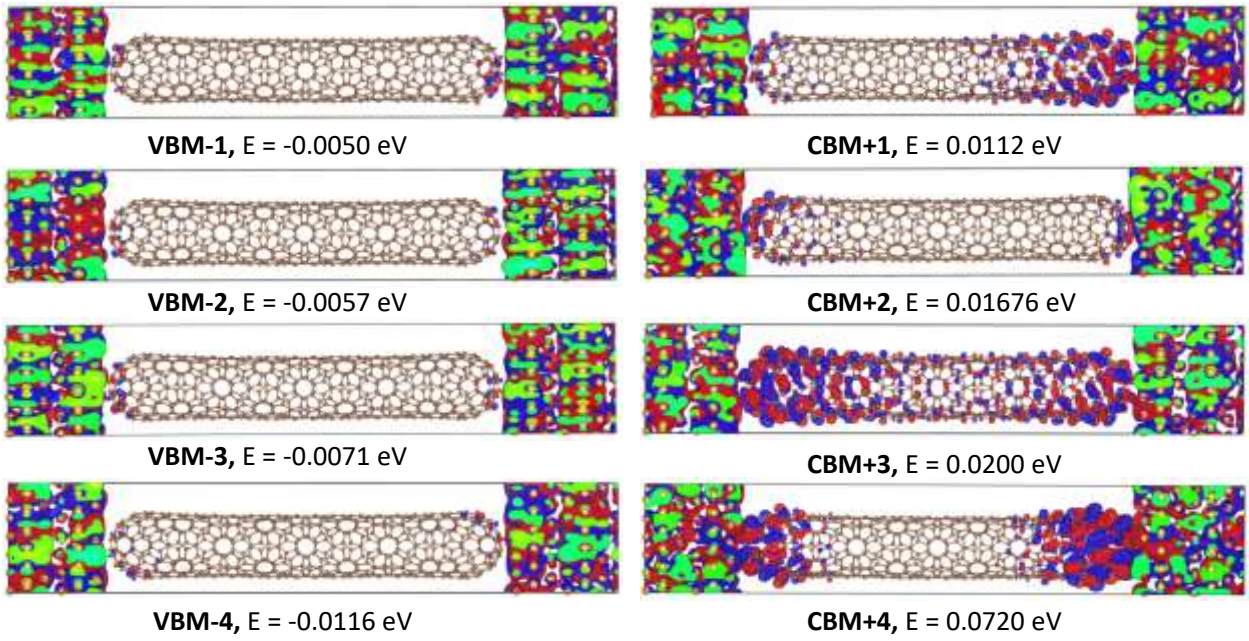

Figure S6: The wavefunctions of Chiral $(8, 4)_S$. The isosurface value is 0.009 electrons/Å^3.

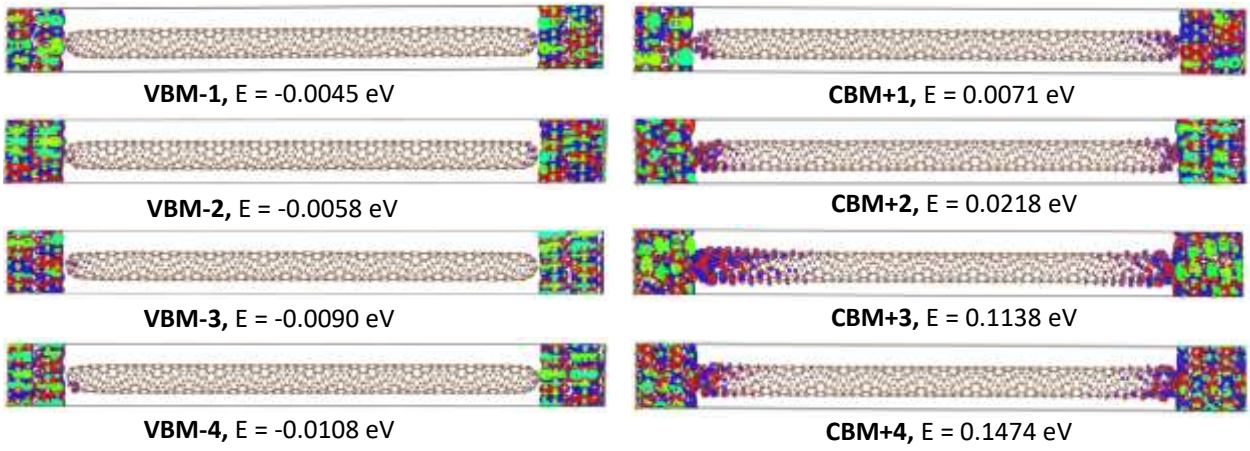

Figure S7: The wavefunction of Chiral $(8, 1)_L$. The isosurface value is 0.009 electrons/Å^3.

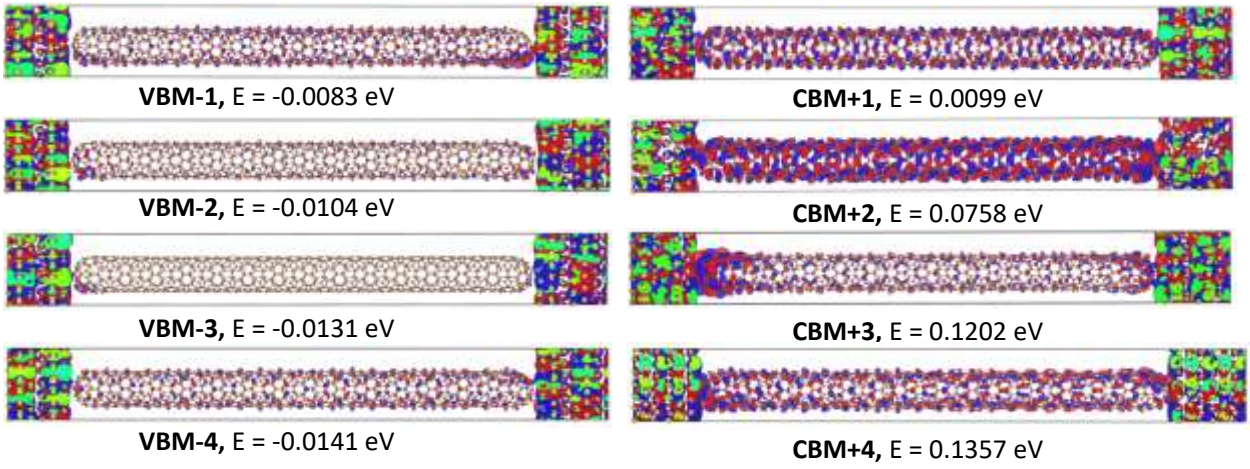

Figure S8: The wavefunction of Chiral $(8, 2)_L$. The isosurface value is 0.009 electrons/Å^3.

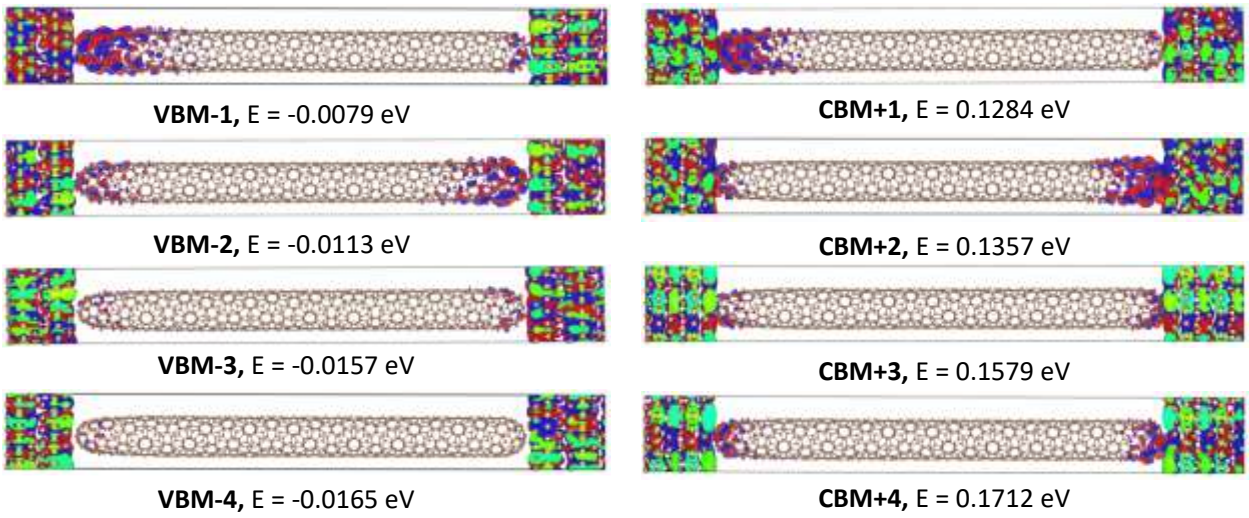

Figure S9: The wavefunction of Chiral $(8, 3)_L$. The isosurface value is 0.009 electrons/Å^3.

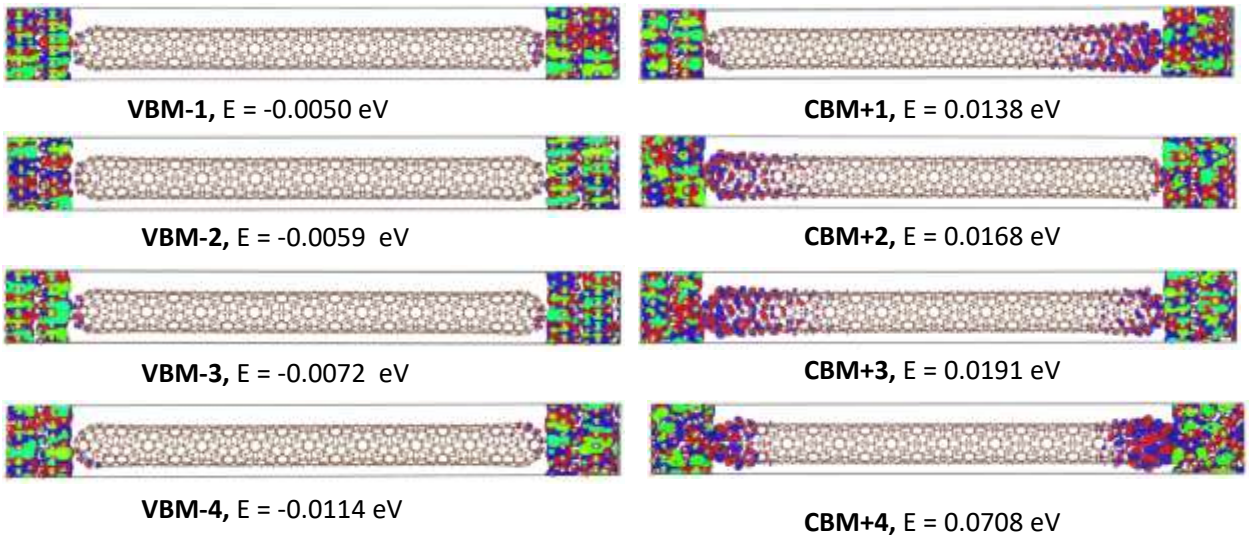

Figure S10: The wavefunction of Chiral $(8, 4)_L$. The isosurface value is 0.009 electrons/Å^3.

4. *I-V* curve (8, *m*)$_{S/L}$

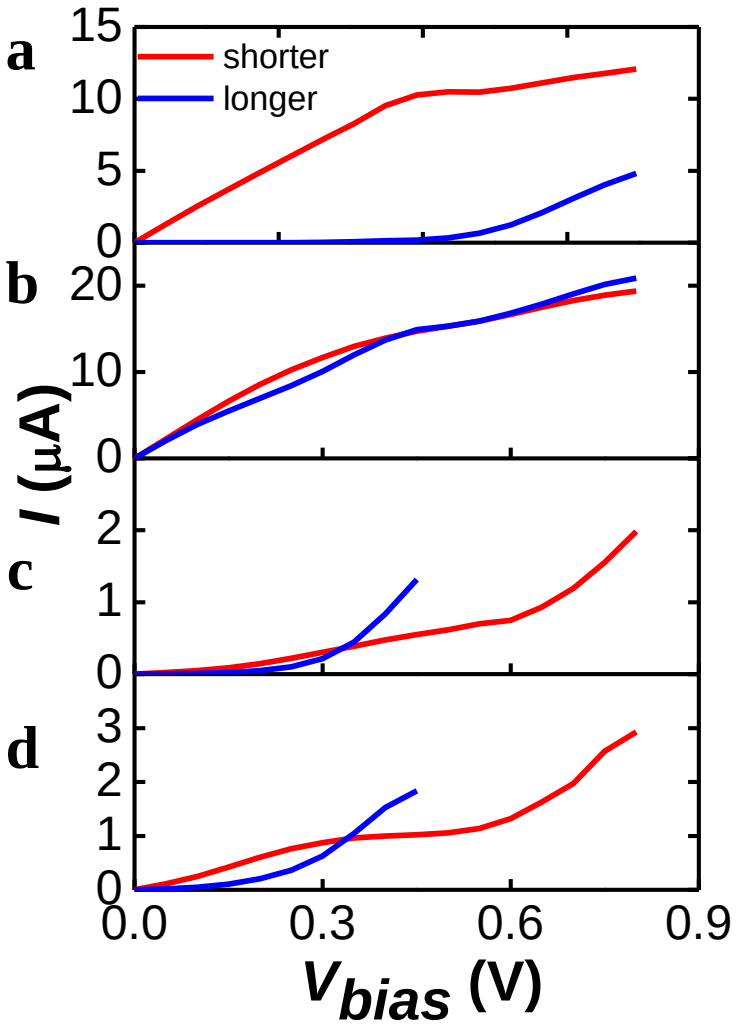

Figure S11. *I-V* curve of chiral (8, 1)$_{S/L}$ (a), (8, 2)$_{S/L}$ (b), (8, 3)$_{S/L}$ (c), and (8, 4)$_{S/L}$ (d) system. Red color shows shorter and blue color shows longer nanotube.

5. DOS of chiral (10, *m*)$_{S/L}$

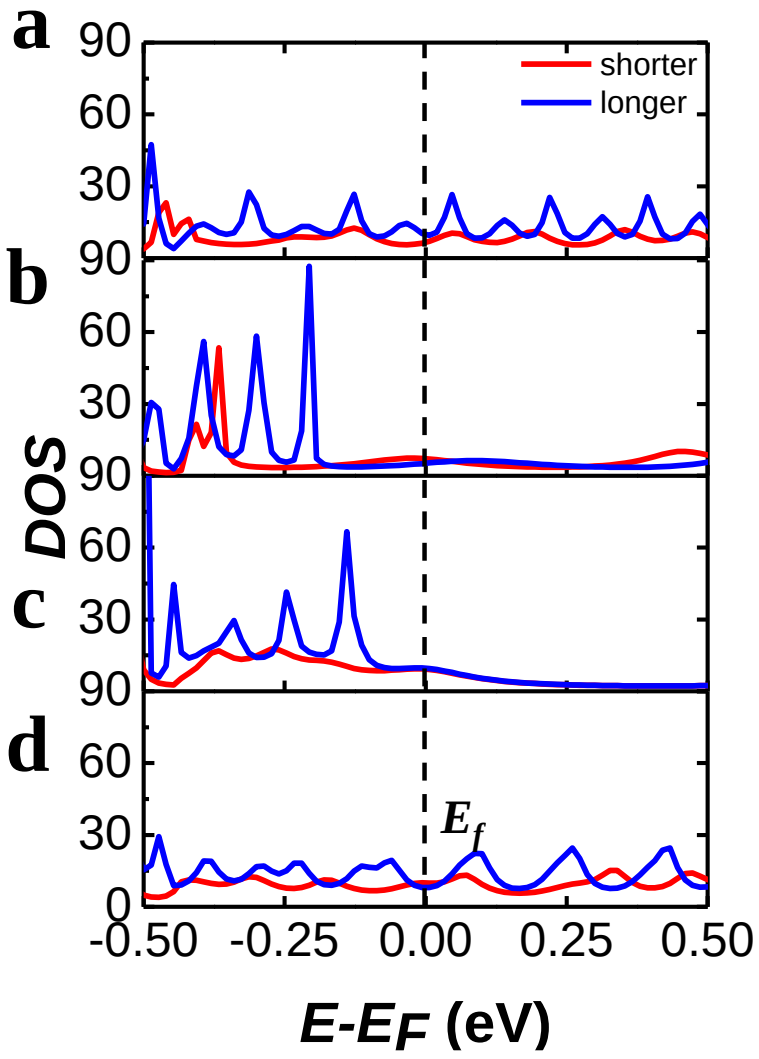

Figure S12. DOS of chiral (10, 1)$_{S/L}$ (a), (10, 2)$_{S/L}$ (b), (10, 3)$_{S/L}$ (c), (10, 4)$_{S/L}$ (d) at zero-bias voltage. Red color shows shorter and blue color shows longer nanotube.

Figure S12 shows the DOS of chiral (10, 1)$_{S/L}$, (10, 2)$_{S/L}$, (10, 3)$_{S/L}$ and (10, 4)$_{S/L}$ with shorter and longer length at zero bias voltage. The DOS of chiral (10, 1) and (10, 4) nanotubes is depicted in Figures S12a and S12d, respectively. Multiple peaks at the E_f are observed in both cases, confirming the metallic characteristics of these nanotubes along both short and long lengths. Figures S12b and S12c show the DOS of chiral (10, 2) and (10, 3) nanotubes. Notably, both shorter and longer nanotubes exhibited a

significant bandgap near the E_f and no electron distribution. This bandgap denoted the semiconducting nature of the system.

6. Wavefunctions of (10, m)$_{S/L}$

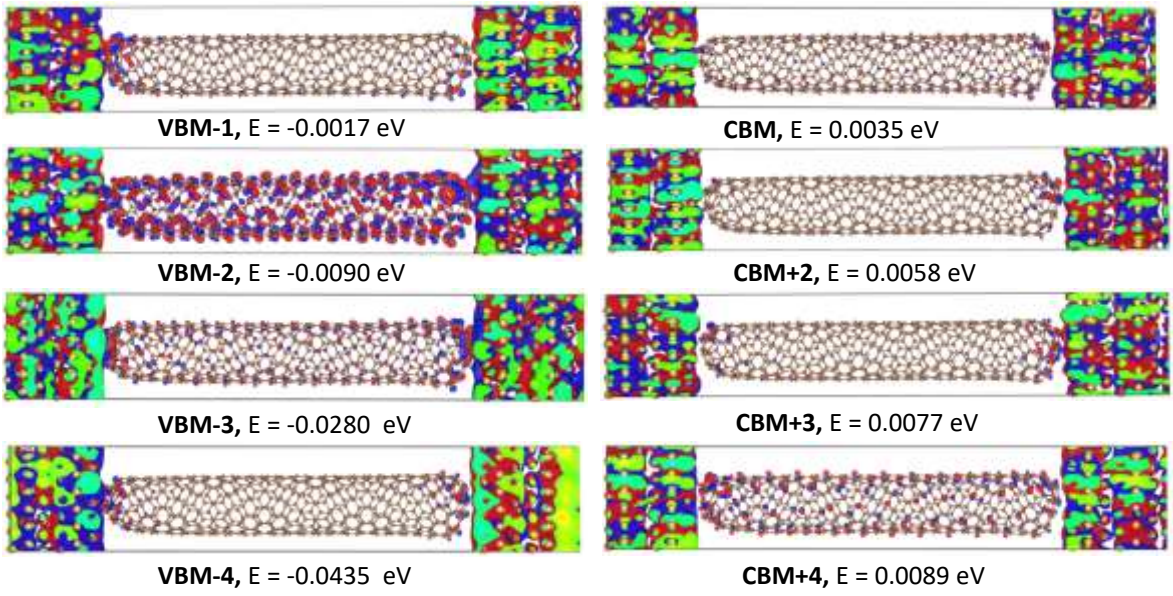

Figure S13: The wavefunctions of Chiral (10, 1)$_S$. The isosurface value is 0.009 electrons/Å^3.

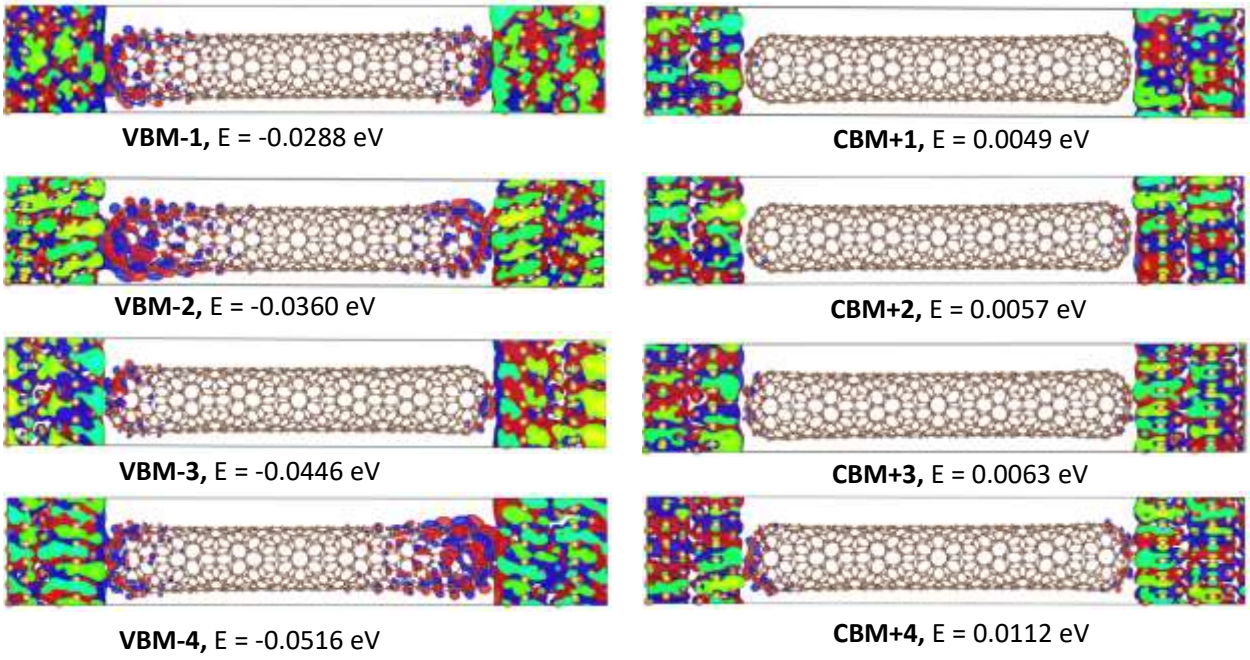

Figure S14: The wavefunctions of Chiral (10, 2)$_S$. The isosurface value is 0.009 electrons/Å^3.

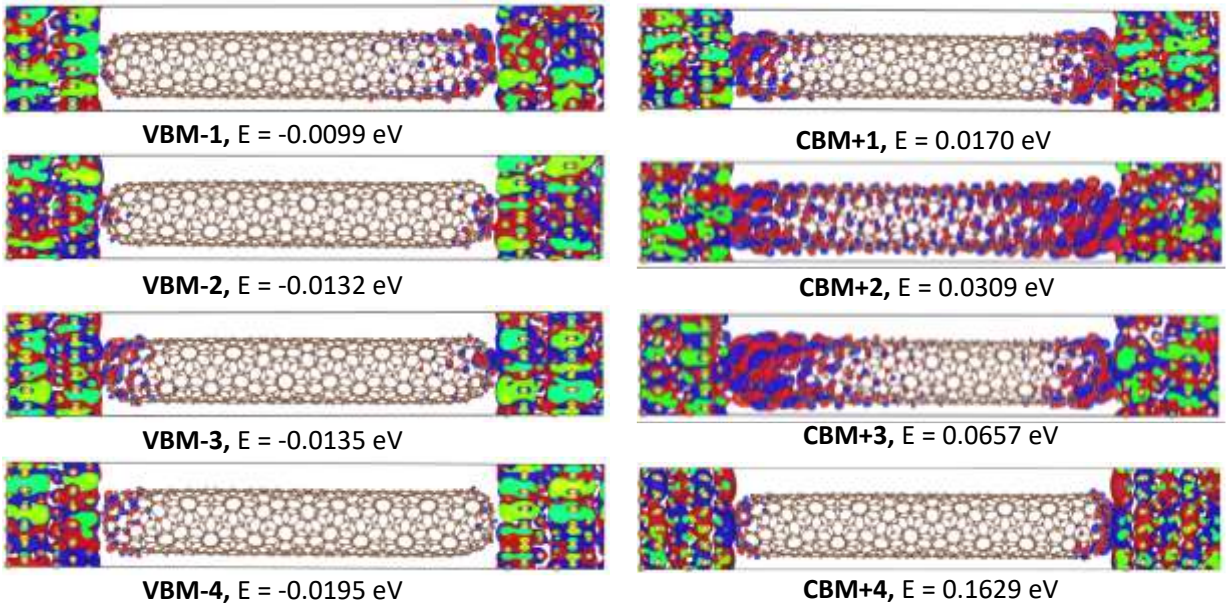

Figure S15: The wavefunctions of Chiral $(10, 3)_S$. The isosurface value is 0.009 electrons/Å^3.

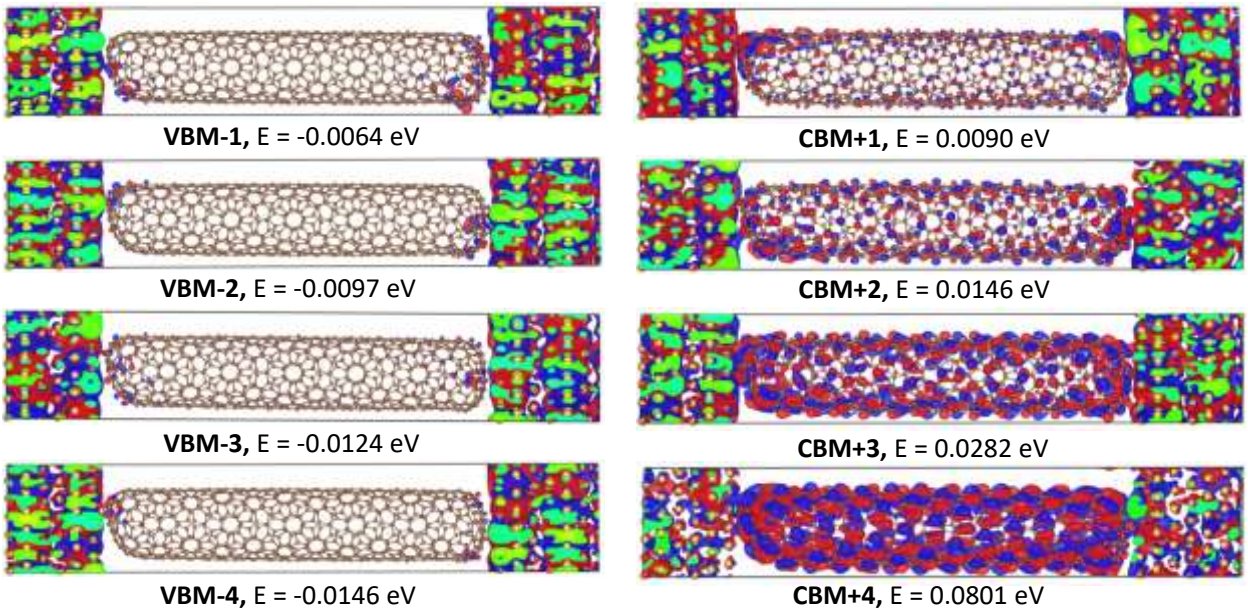

Figure S16: The wavefunctions of Chiral $(10, 4)_S$. The isosurface value is 0.009 electrons/Å^3.

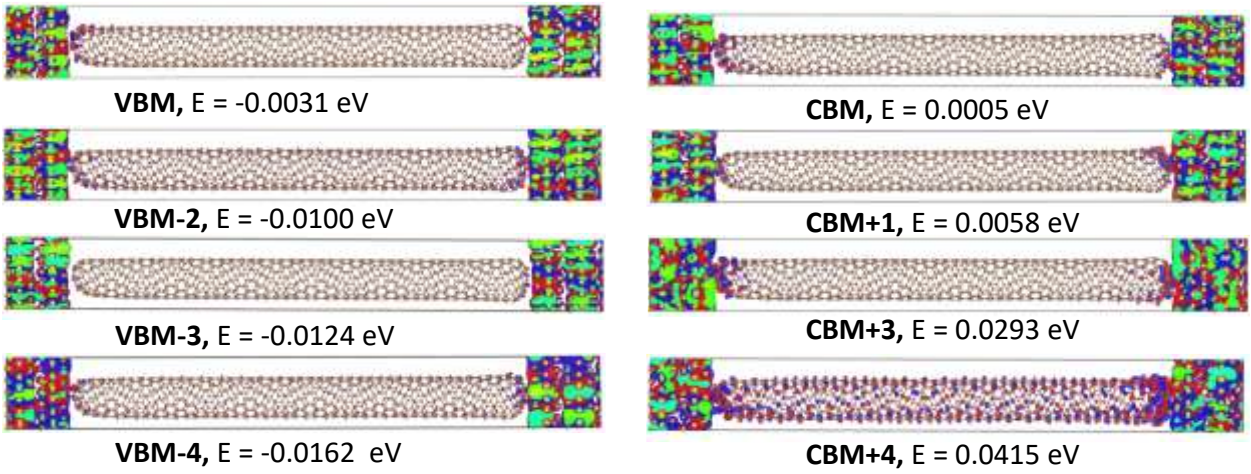

Figure S17: The wavefunctions of Chiral $(10, 1)_L$. The isosurface value is 0.009 electrons/Å^3.

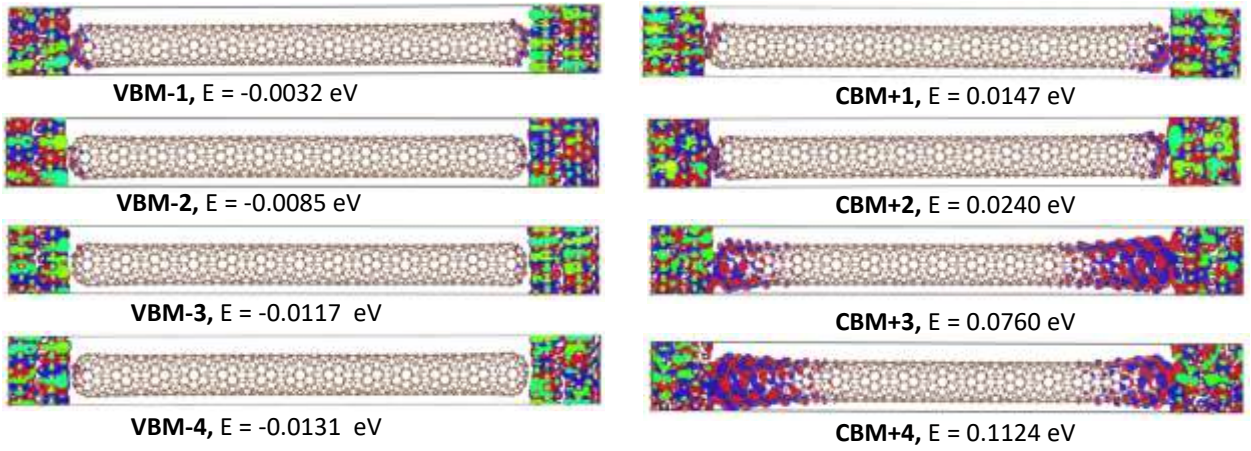

Figure S18: The wavefunctions of Chiral $(10, 2)_L$. The isosurface value is 0.009 electrons/Å^3.

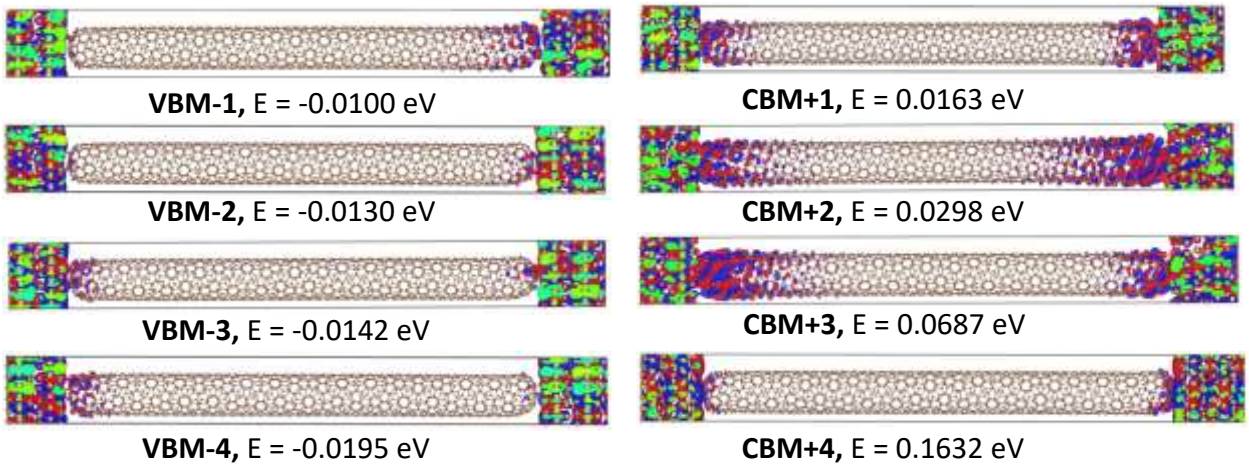

Figure S19: The wavefunctions of Chiral $(10, 3)_L$. The isosurface value is 0.009 electrons/Å^3.

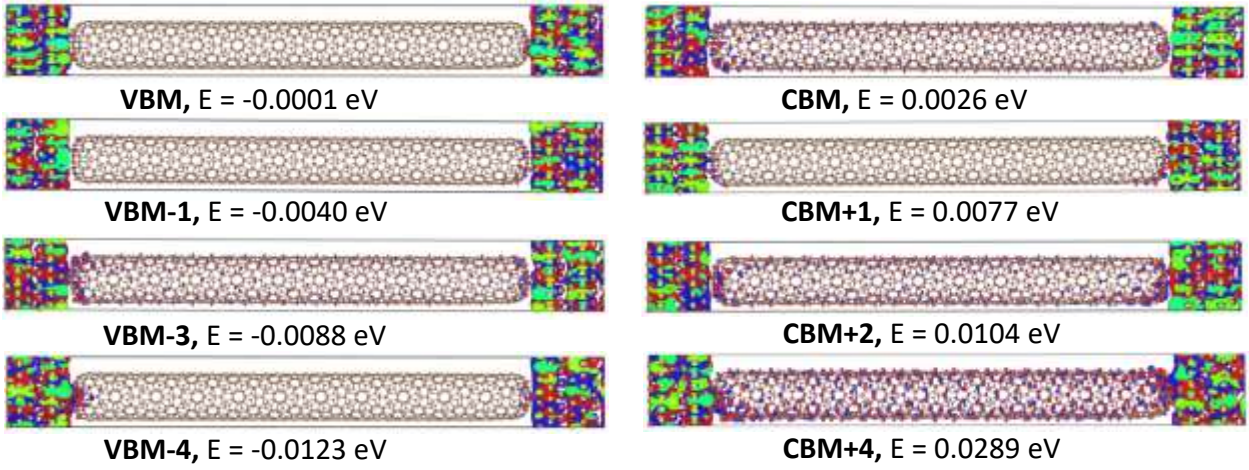

Figure S20: The wavefunctions of Chiral $(10, 4)_L$. The isosurface value is 0.009 electrons/Å^3.

7. *I-V* curve of chiral (10, *m*)$_{S/L}$

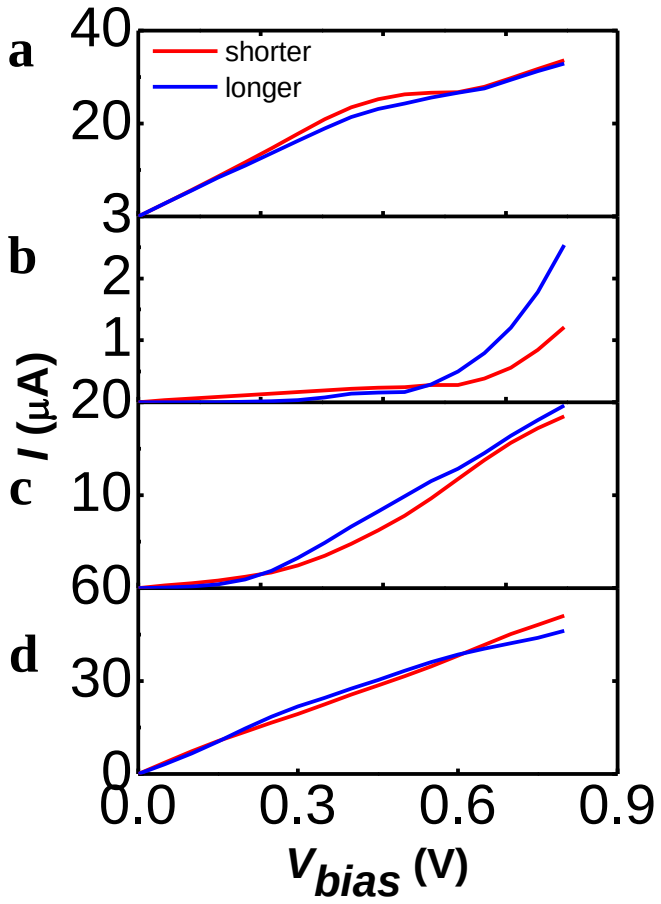

Figure S21. *I-V* curve of chiral (10, 1)$_{S/L}$ (a), (10, 2)$_{S/L}$ (b), (10, 3)$_{S/L}$ (c), and (10, 4)$_{S/L}$ (d) system. Red color shows shorter and blue color shows longer nanotube.