Supporting Information

Pseudo-potential energy at crossed CNT junction

The structure distortion of CNTs and the separation gap between CNTs d_{gap} can be determined by minimizing a pseudo-potential energy at the crossed CNT-CNT junction. Effected by the bending of both neighboring CNT walls, the total pseudo-potential energy, E, of the junction can be expressed by

$$E = \begin{cases} 0 & \text{if } d \geq D + d_{vdw} \\ 2E_b + E_{LJ} & \text{if } d < D + d_{vdw} \end{cases} \qquad \text{(S1)}$$

where E_b is the bending energy of neighboring CNT walls and E_{LJ} is the energy associated with the Van der Waals interaction between CNTs, respectively.

Assume the energy associated with the bending of CNT walls can be represented by a harmonic potential as

$$E_s = \frac{1}{2} k_s \left(D - D'\right)^2 \qquad \text{(S2)}$$

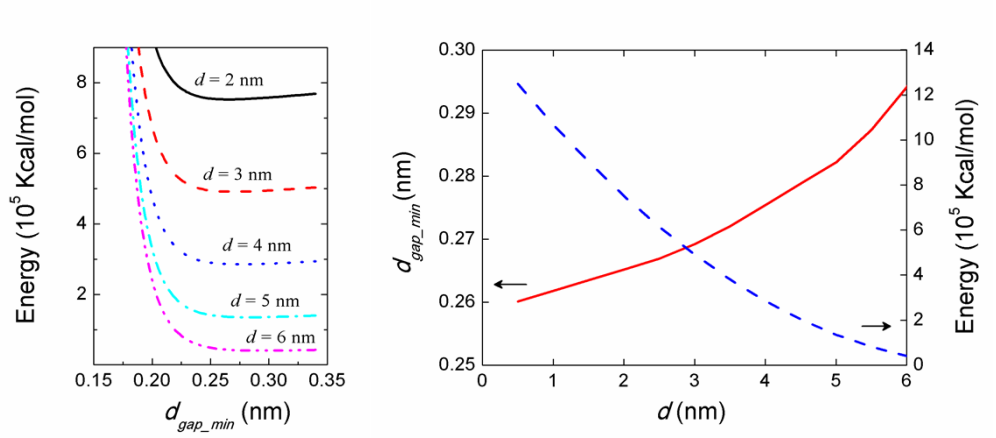
where D is the diameter of CNT before distortion, D' is the nominal diameter of distorted CNT, k_s is the equivalent spring constant of CNT walls. The spring constant can be derived from the atomic dynamic simulations by keeping one CNT fixed, while slowly moving another CNT towards the fixed one in the radial direction. As two CNTs are radially compressed, we can calculate the force-deformation curve by the coarse-grained molecular dynamic model and derive the spring constant k_s accordingly.

The potential energy associated with the Van der Waals interaction is represented by the Lennard-Jones potential,

$$E_v = 4k_v\left[\left(\frac{\sigma}{d_{gap}}\right)^{12} - \left(\frac{\sigma}{d_{gap}}\right)^{6}\right] \qquad \text{(S3)}$$

where k_v is the depth of the potential well obtained from the atomic dynamic model, σ is the finite distance at which the potential is zero.

Figure S1 shows the typical characteristics of the pseudo-potential energy of a SWCNT junction, where the diameter of CNT is D = 6.9 nm, the equivalent spring constant of CNT is k_s = 1.12 × 10^5 kcal/(mol·nm^2), the depth of the potential well of the Lennard-Jones potential is k_v = 92 kcal/mol, and the constant σ = 0.3029 nm corresponds to a zero Lennard-Jones force at the Van der Waals distance of undeformed CNT, such that, $\partial E_v / \partial d'_{\mathrm{vdw}}\big|_{d'_{vdw}=d_{vdw}=0.34nm} = 0$. It can be seen from Figure S1(a) and S1(b) that the total pseudo-potential energy of a CNT-CNT junction has a minimum value for every given d, which corresponds to a balanced distance d_{gap_min} between the walls of two distorted CNTs. As the distance d between CNTs decreases, the minimum pseudo-potential energy increases due to the increased CNT wall distortion and, correspondingly, the distance d_{gap_min} decreases. The distance d_{gap_min} in the effective contact/tunneling region of two CNTs reaches an extreme at near 0.26 nm from our model. Any further decrease in distance d between CNTs will result in the bending of CNT wall over a larger area rather than further decreasing the distance d_{gap}.



(a) (b)

Figure S1. Pseudo-potential energy values vs. CNT-CNT distance d. (a) Variation of total potential energy vs. d_{gap_min} at different distance d. (b) Variations of total minimum potential energy and d_{gap_min} vs. distance d.