Supporting Information

A Polythiophene-SWCNTs Assembled Nanorobot to Clean Up Gas Molecules

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1. H_2 release upon increasing the length of PT chains

The dependence of hydrogen release on chain length is studied by introducing four groups of PT chains with different lengths into the system. For comparison, the total molecular weight of each PT chains group is set to be approximately equivalent by assigning different chain numbers. For instance, the molecular weight of 24 PT5 chains corresponds to that of 8 PT15 chains. The snapshots of residual hydrogen configurations are summarized in Figure S1 for different chain lengths when the simulation systems reach equilibration at 300 K and 10 MPa. It is observed that the amount of residual H_2 molecules attached to (10, 10) SWCNT increases with the chain length increasing. As demonstrated in Figure S2a, the hydrogen release ratio expresses a downward trend with respect to the increasing chain length. This trend of hydrogen release ratio is mainly attributed to the different amounts of binding cells between PT chains and SWCNT surfaces, which are directly reflected by the PT chain's binding energies with the tube in Figure S2b.

These four groups of PT chains are constructed with an identical number of primitive cells, which means that they would show comparable binding energy with the SWCNT in their respective systems assuming that all these PT cells are sufficiently bounded to the tube surfaces. Nevertheless, it is not occurred along with the time-evolution of interaction energy profiles between PT chains and the tube (Figure S2b). With the same total amount of 120 PT cells, PT5 system shows the highest binding energy with the tube. This higher binding energy represents a more sufficient combination between PT chains and SWCNT, promoting a more effective hydrogen release by reducing the H_2 storage space on the tube surfaces (Figure S1e). Therefore, the highest hydrogen release ratio is achieved in PT5 system (Figure S2a). Similarly, the lowest hydrogen release ratio is obtained in PT20 system which exhibits minimal binding energy with the tube since nearly half of the PT20 chains are not effectively interacted with SWCNT, as shown in Figure S1h.

Furthermore, it is observed that the hydrogen release performance of both PT10 and PT15 systems is inferior to that of the PT5 system, though their binding energy values between PT chains and SWCNT are comparable to that of the PT5 system. This indicates that the binding energy between PT chains and SWCNT is not the only parameter determining the hydrogen release ratio of the system. Moreover, the hydrogen release performance of PT10 system is slightly superior, while the binding energy in PT10 system is a little lower than that of PT15 system. It is mainly owing to the different amounts of PT chains with the same total molecular weight in their respective systems. Apart from the binding interaction between PT chains and SWCNT, the vdW interaction at both ends of PT chains would also occupy extra space on SWCNT surfaces to release H_2. When the number of PT chains is significantly large, this PT_{ends} vdW interaction would have a conspicuous impact on the hydrogen release performance. Therefore, due to the contributions from both PT-SWCNT binding space and PT_{ends} vdW interaction space, the hydrogen release ratio in PT5 system is the highest one, followed by PT10, PT15, and PT20 systems in turn.

Though the highest release ratio of about 82.5% is obtained by introducing PT5 chains into the hydrogen storage system, it is hard for SWCNT to capture such a large number of chains in a short while. As shown in Figure S2b, there is a pseudo equilibration time of about 0.75 ns during which several PT chains have no interaction with the tube. Afterward, it takes about 0.55 ns for chains to be gradually captured and adjust their positions to reach equilibration. The equilibration time for the PT5 system is nine times than that of the PT15 system. Among these systems, PT15 system exhibits a relatively high hydrogen release ratio in the least time. To completely release the absorbed hydrogen in a rapid way, PT chains, a bit longer than (10, 10) SWCNT, are preferred to be applied into the storage system in the case of sufficient PT chains. Hence, it is appropriate to investigate the amount effects of PT chains on the performance of hydrogen release based on PT15 chains in this work.

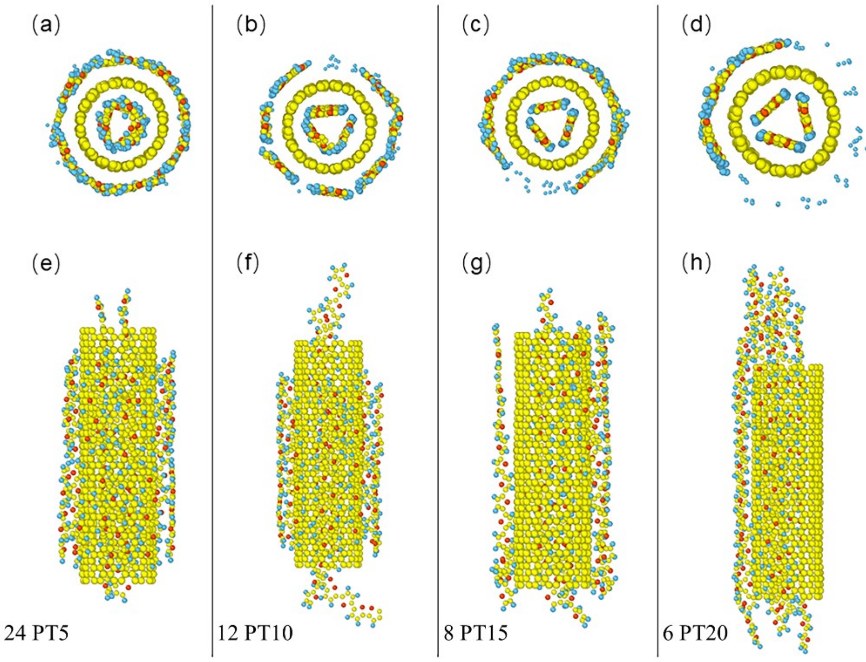

Figure S1. (a-d) The final snapshots (end face of tubes) of the top view and (f-h) side view with respect to different chain lengths.

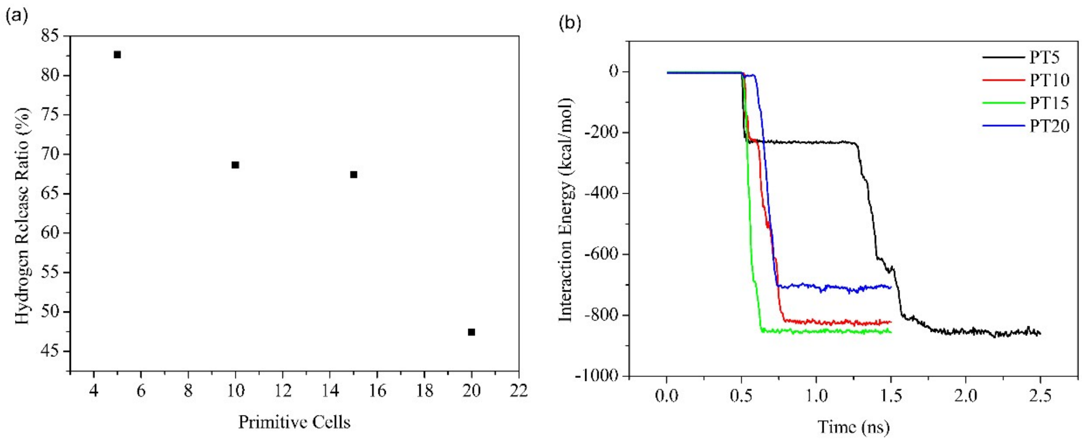

Figure S2. (a) Hydrogen release ratios and (b) time evolution of the interactions between (10, 10) SWCNTs and PT chains with different primitive cells.

2. The PT chains were dragged away from SWCNTs surfaces.

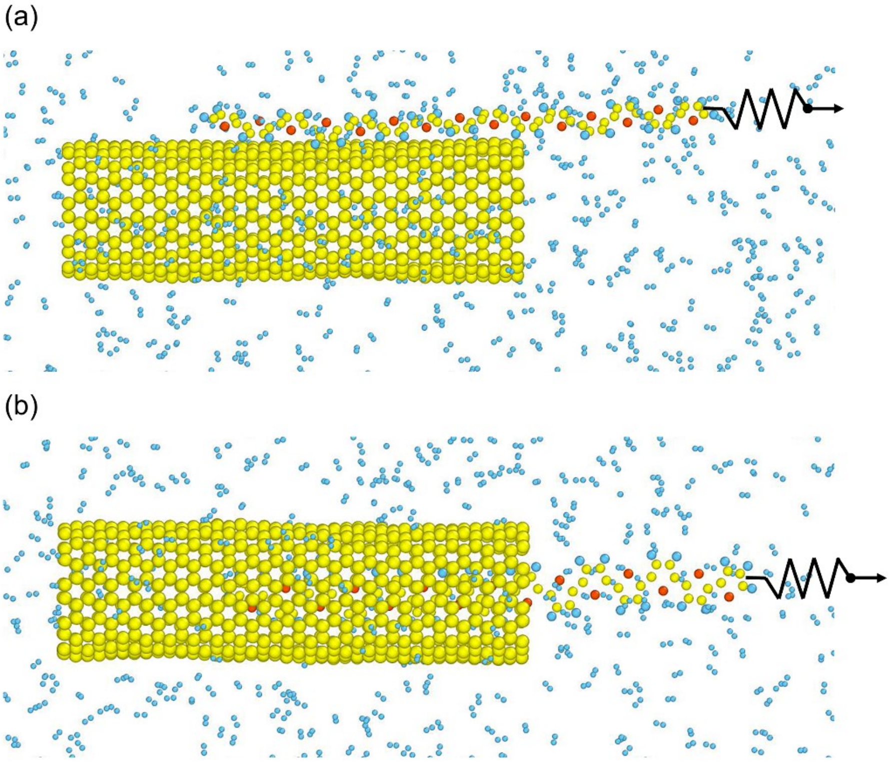

Figure S3. The PT chains were dragged at a constant moving speed by a virtual spring away from SWCNTs surfaces.

3. The derivation of equations (2) and (3)

As shown in Fig S4, the red line represents the carbon skeleton of the PT chain, and l_{AB} denotes the width of the carbon skeleton. To simplify the calculation and make compensation for the influence of hydrogen atoms to some degree, we take the approximate skeleton width as 3.4 Å. The van der Waals diameter (l_{BC}) for carbon atoms is 3.4 Å as well.

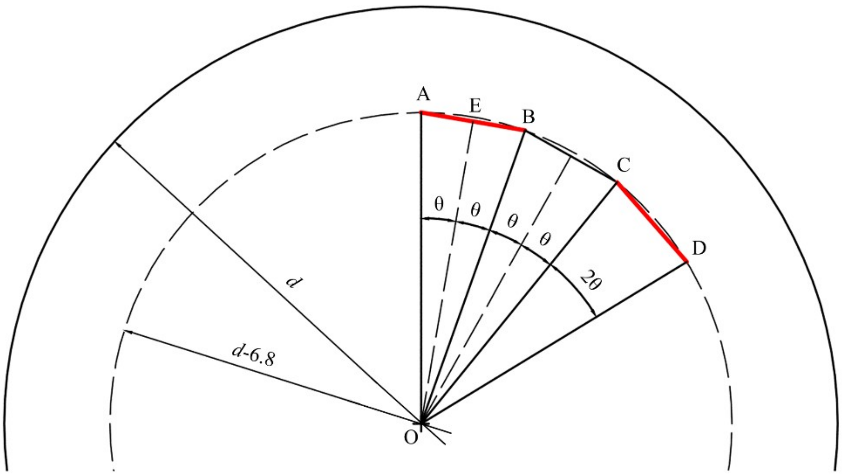

Figure S4. Schematic diagram of PT chain arrangement inside the tube. The outer circle denotes the carbon tube with a diameter of *d*. The inner circle is an imaginary circle with a diameter of (*d*-6.8). AB and CD denote the cross-section of the carbon skeleton of the PT chain. A, B, C, and D are points on the inner circle. O is the center of both circles and E is the midpoint of AB. The size of angle AOE is *θ*. The unit of length is Å.

For SWCNTs in the diameter range of 10-20 angstrom, due to the orderly arrangement of PT chains on the tube surface, the amount of PT chains inside the tube can be derived from the following equations

$$\sin\theta = \frac{l_{AE}}{l_{OA}} \tag{3}$$

$$\theta = \arcsin\left(\frac{l_{AE}}{l_{OA}}\right) \tag{4}$$

$$N_{in} = \frac{360}{4\theta} = \frac{90}{\theta} = \frac{90}{\arcsin\left(\frac{l_{AE}}{l_{OA}}\right)} = \frac{90}{\arcsin\left(\frac{3.4}{d-6.8}\right)} \tag{5}$$

In the same way, the amount of PT chains outside the tube can be obtained:

$$N_{out} = \frac{90}{\arcsin(\frac{3.4}{d+6.8})} \quad (6)$$

where N_{in} and N_{out} are the amounts of PT chains inside and outside the tube respectively, and d is the diameter of SWCNTs. l_{AE} denotes half the width of the carbon skeleton. l_{OA} denotes the radius of the imaginary circle.