Supplementary Information

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S1. Computational details

Theoretical calculations are performed by the ab initio code package Atomistix ToolKit (ATK-VNL). ATK-VNL is a modeling and simulation platform on atomic scale that combines a great deal of methods and models. It is an easy-to-operate graphical interface, which makes tasks easy to perform. Therefore, it can effectively execute complex workflows and perform high-level data analysis.

For the electronic structure optimizations and electronic band structure calculations the k-points is set to be 1×1×15. And for the calculations of electronic band structure, the lengths of these BAs nanotube unit cell (along 1D direction) with periodic boundary condition are 6.66 Å (96 atoms).

But for the devices, the scattering region is not periodic in the electron transport direction. Since the system has no periodicity in z-direction (electron transport direction), one should therefore not need more than one k-point in this direction. We do, however, need k-point sampling in all directions for the electrodes. These are still assumed to be periodic in z-direction, and the electronic states of the electrodes are obtained from a standard bulk calculation, with k-points in all directions.

In this manuscript, we make an ideal system that the electrodes are identical to the central region. Let HL, HCR, and HR be the Hamiltonians of the left electrode, central region, and right electrode, respectively. HL and HR are calculated under periodic boundary conditions, while HCR is evaluated with open boundary conditions using self-energies obtained from HL and HR. Now, clearly you will only get perfect transmission in this system if HL=HR=HCR. To obtain this, the same k-point sampling should be used in the x and y directions in the electrodes and in the open boundary condition calculation for the central region. This point is quite trivial, and must always be obeyed in a calculation. The actual number of kx, ky points required is a matter of balancing performance vs. accuracy, just like for any other calculation.

In the z-direction, the self-energy calculation effectively corresponds to an infinite number of k-points, and you will need a lot of kz-points in the electrode calculation to match the electronic structures of the electrodes and the central region. The primary quantity that needs to be closely matched is the Fermi level. A difference here will lead to slow or bad SCF convergence, and in the

worst case inaccurate results. The ATK default value of kz = 100 is probably quite far on the safe side. But it is relatively inexpensive since these k-points are only used in the electrode calculation, which is the smaller and faster part of the full computation.

S2. Calculation Results

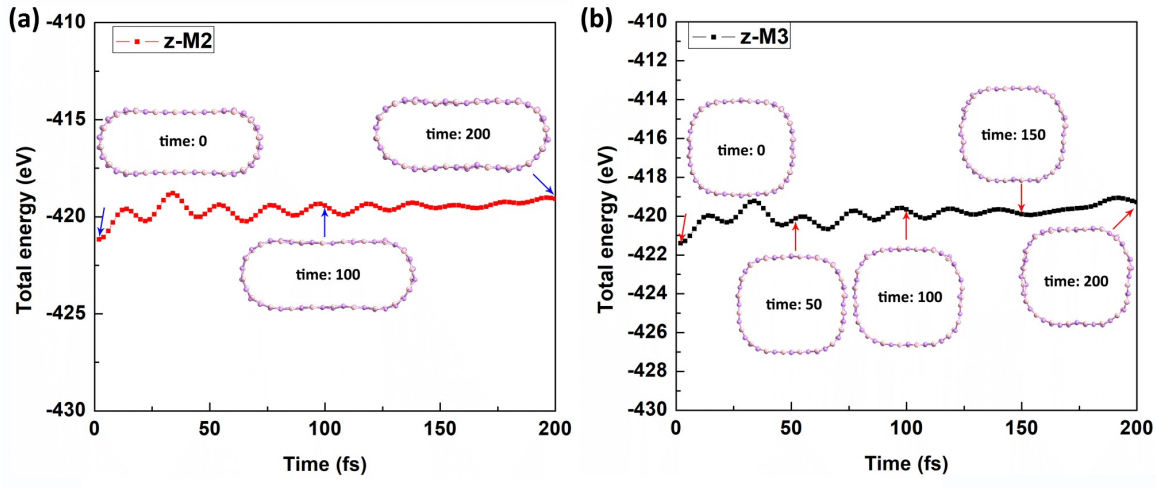

Fig. S1. Time-varied total energy of the zigzag BAs nanotubes with (a) elliptical and (b) square cross-section shapes.

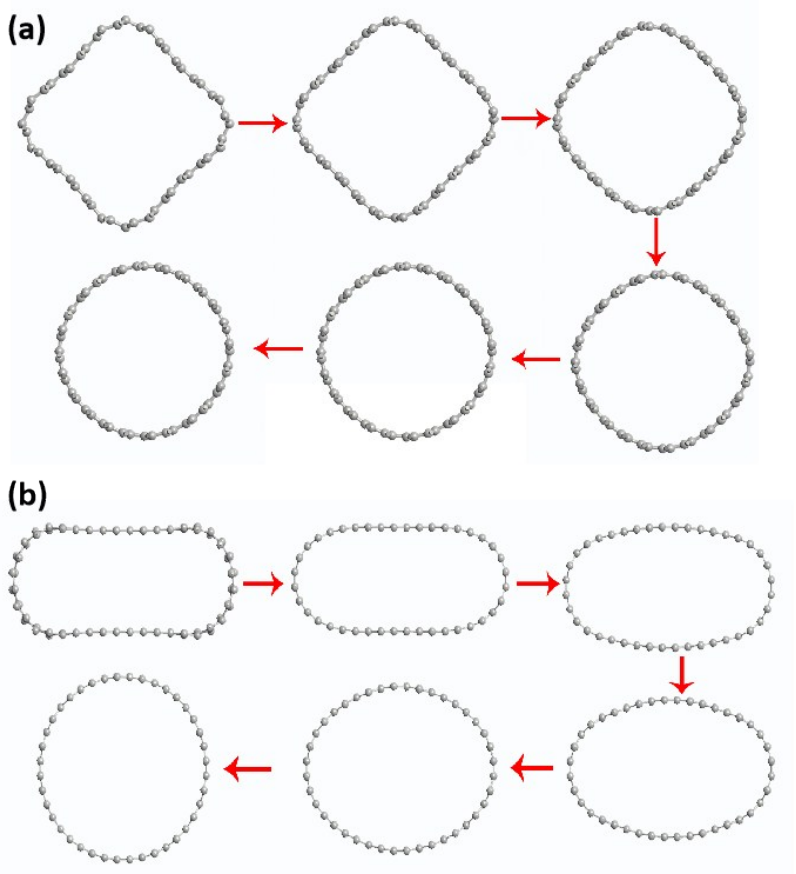

Fig. S2. The atomic structures of the (a) square and (b) elliptical CNTs before and after optimization.

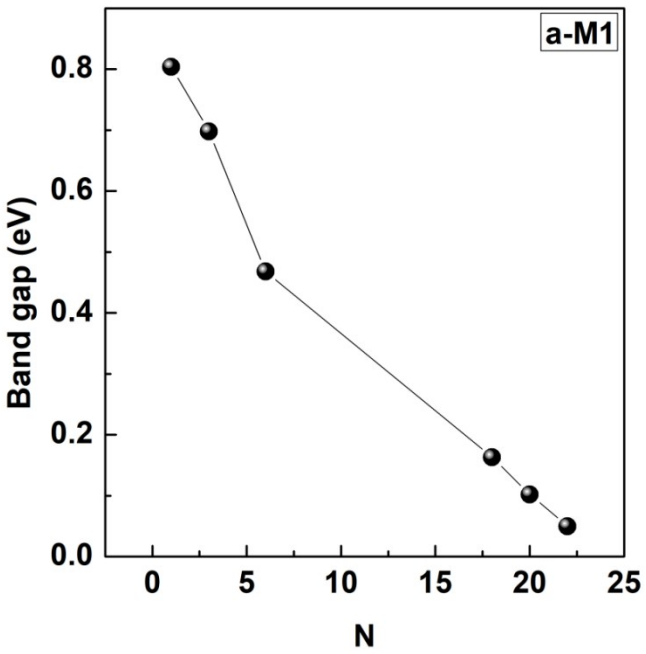

Fig. S3. Band gap-numbers of H_2O molecules encapsulated in a-M1.

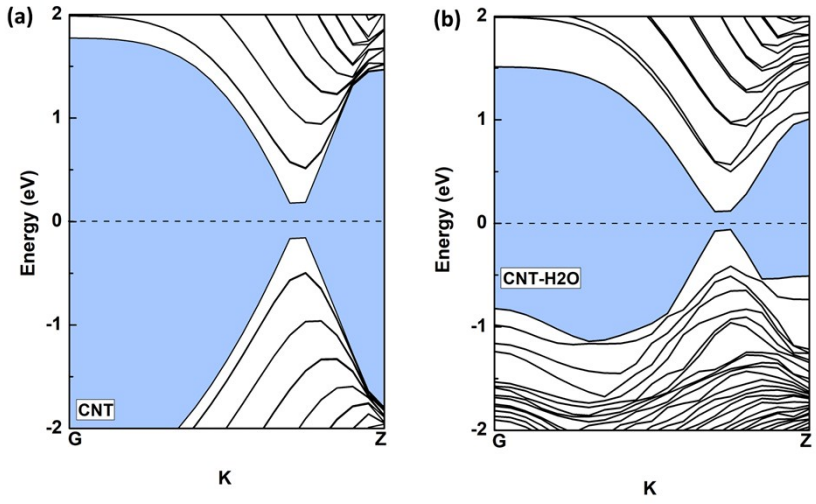

Fig. S4. Electronic band structures of the circular CNT (a) before and (b) after the encapsulation of H_2O.