Supporting information for "Nanopore Sensor for Detecting Nanotoxicity of a Carbon Nanotube to Proteins"

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Simulation set-up

The simulated system was first equilibrated at 1 bar and 300 K for 5 ns. During the equilibration, backbone atoms in the CNT-WW complex (60-Å away from the pore opening, was constrained. The equilibrated system measures 85×85×178.5 $Å^3$. Subsequent simulations, with various biasing voltages, were carried out in the NVT ensemble. Atoms in the solid membrane were harmonically constrained to their original positions in all simulations, so the solid membrane can not move. The Langevin dynamics was applied to all atoms in the solid to keep the temperature in a simulated system to be constant. We used the TIP3P model for water[1], standard ion force field[2] and silica force field[3] for the solid membrane. The force field for the CNT-protein complex is same as in ref.[4]. A smooth cutoff (10-12 Å) was used to calculate van der Waals energies. Electric interactions were calculated using the particle-mesh Ewald (PME) method (grid size ~ 1 Å). The integration time-step in a simulation was 1 fs.

Current traces for the complex translocation through the solid-state nanopore

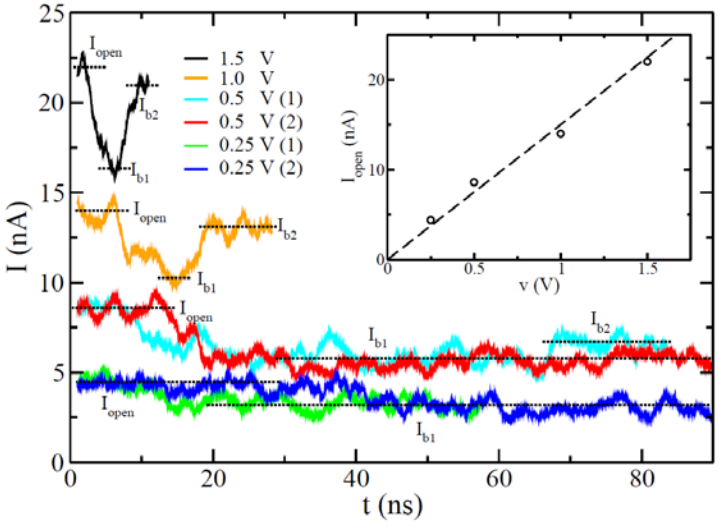

Figure S1 Traces of ionic currents for translocation of the complex through the nanopore. Inset: open-pore currents vs. biasing voltages.

Figure 1b and 1c in the paper show current traces for the complex translocation at a biasing voltage of 0.5V. In Fig. S1, we provide current traces for 0.25, 1.0 and 1.5 V as well. When the biasing voltage is 0.25 V, only one level of current blockage (I_{b1}) is present in two independent simulations. This indicates that the CNT-WW complex was stuck inside the pore. At a voltage of 0.5 V or larger, two levels of current blockages (I_{b1} and I_{b2}) are observed. The second level of blockage (I_{b2}) occurs after the rupture of the complex, i.e. the CNT was driven through the pore and the protein was left on the pore surface.

The inset of Figure S1 show that the open-pore current increases linearly with the biasing voltage. The slope of the fitting line (dashed) yields the conductance *S* (in a 1M electrolyte) of the pore used in simulations. Thus, $S = I/V = 14.6$ nS.

Ionic screening of a charged CNT

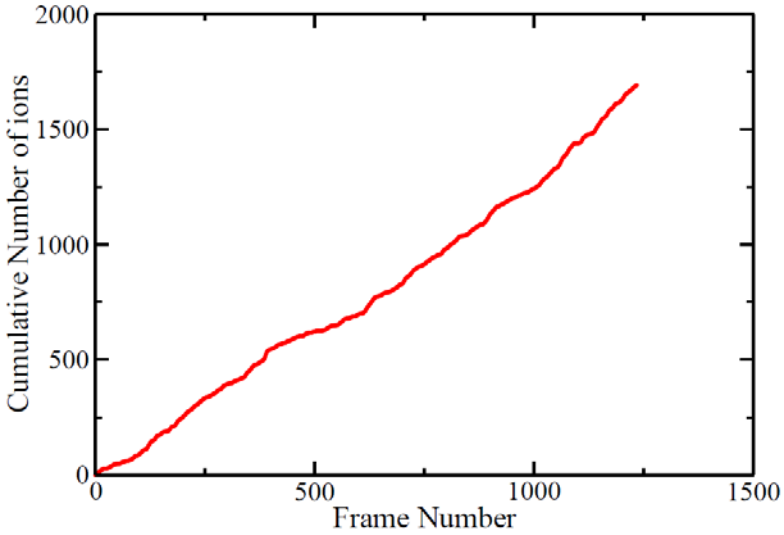

Figure S2. Cumulative number of counter ions within 3 Å of the charged part of the CNT. The time interval between two frames is 10 ps.

After the complex was immobilized inside the pore, the CNT was pulled in the biasing electric field and was hold by the protein molecule (WW domain) in the meanwhile. The complex was stable as long as the electric driving force is less than the contact friction force between the CNT and the protein molecule. At a biasing voltage of 0.25 V, the complex was stable in the pore. From the simulation trajectory (~ 12.5 ns), we computed number of counter-ions within 3 Å (the Debye length for a 1 M electrolyte) of the charged part of the CNT. Co-ions are barely present in that region. Figure S2 shows the cumulative number of those ions and the mean slope of the line yields the time-average number (~ 1.4) of counter-ions that screen the CNT's charge. Therefore, the effective charge (because of ion screening) of the CNT is 86% of the total charge of the bare CNT.

Movies

1) The movie file named 05V.mpg illustrates that the complex was driven towards the pore at a biasing voltage of 0.5 V and was struck inside the pore thereafter.

The nanopore and the solid membrane are in a cross-section view. K^+ and Cl^- ions are colored in tan and cyan. Atoms in the CNT-WW complex are shown as van der Waals spheres. Simulation time is about 25 ns.

2) The movie file named 1V.mpg illustrates that the complex was driven towards the pore at a biasing voltage of 1 V, followed by a rupture of the complex inside the pore. After the rupture, the CNT was further electrically driven through the pore and the protein molecule was stuck on the pore surface. The nanopore and the solid membrane are in a cross-section view. K^+ and Cl^- ions are colored in tan and cyan. Atoms in the CNT-WW complex are shown as van der Waals spheres. Simulation time is bout 19 ns.

References

(1) Jorgensen, W. L.; Chandrasekhar, J.; Madura, J. D.; Impey, R. W.; Klein, M. L. *The Journal of chemical physics* **1983**, *79*, 926.

(2) Beglov, D.; Roux, B. *The Journal of chemical physics* **1994**, *100*, 9050.

(3) Cruz-Chu, E. R.; Aksimentiev, A.; Schulten, K. *The Journal of Physical Chemistry B* **2006**, *110*, 21497-21508.

(4) Zuo, G.; Huang, Q.; Wei, G.; Zhou, R.; Fang, H. *ACS Nano*, *4*, 7508-14.