Supporting Information

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SI Text

Fig. S1 and Movies S1 and S2 show details on how the external charge determines the dipole orientations within the Y-SWNT (see main text). Fig. S2 shows the extra simulation results with 2 additional water models, TIP4P and SPC/E. Our results show that the transduction capability of the Y-shaped carbon nanotubes is very robust. Fig. S3 shows the additional simulation results with a T-shaped tube. Our results show that the transduction capability of water-mediated signal is insensitive to small angular changes.

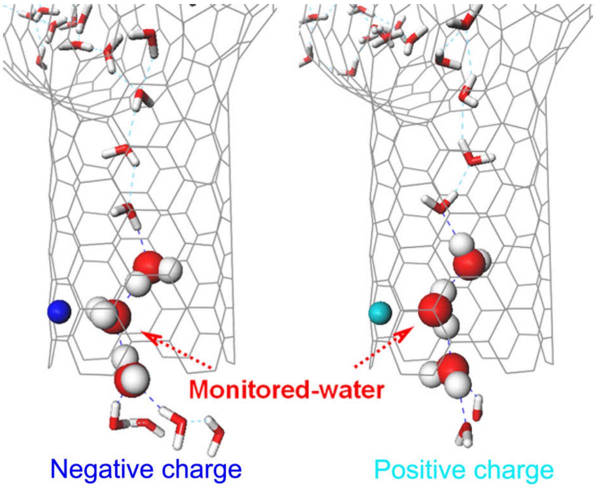


Fig. S1. Water orientations and configurations near the external charge. The external charge $q = -e$ attracts both hydrogen atoms of the monitored water molecule as previously described. The O atom of the monitored water strongly attracts an H atom of the water molecule just above the monitored water molecule, resulting in a downward orientation of the water molecule. This induces group-wise downward orientations of all of the water molecules above the monitored water in the main tube. Conversely, when $q = +e$, the external charge attracts the O atom of the monitored water. One of the H atoms of this monitored water points upward, resulting in an upward orientation of the water molecule just above the monitored water. This gives upward dipole orientations to all of the water molecules above the monitored water in the main tube.

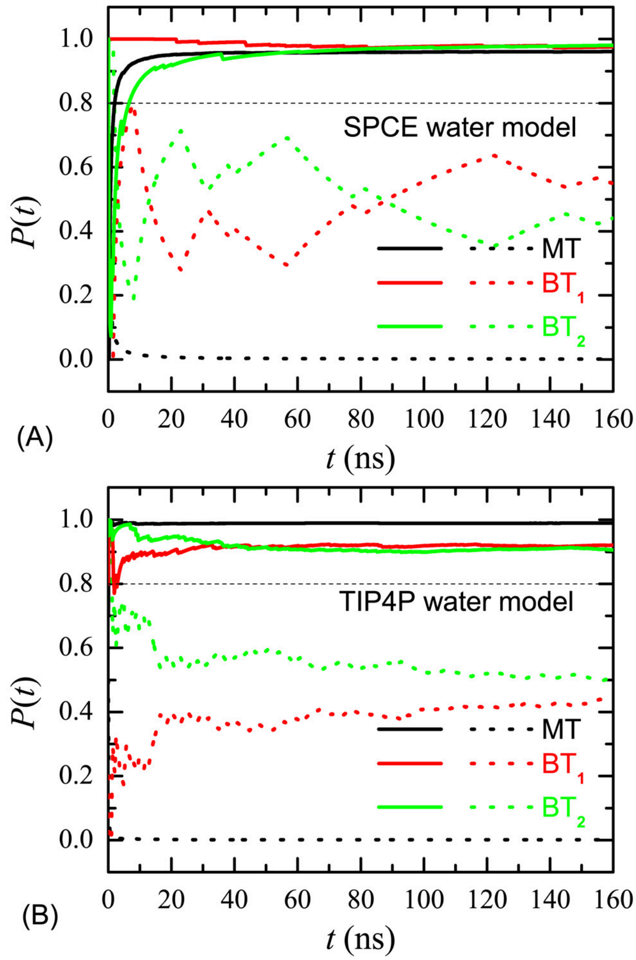


Fig. S2. The probability $P(t)$ of water dipole orientation in a Y-shaped carbon nanotube with different water models. The probability for a negative charge signal is shown in solid lines and probability for a positive charge in dashed lines. (*A*) SPC/E water model; (*B*) TIP4P water model. Results from various water models basically show the same conclusion for the water dipole orientation preferences and water-mediated signal transduction.

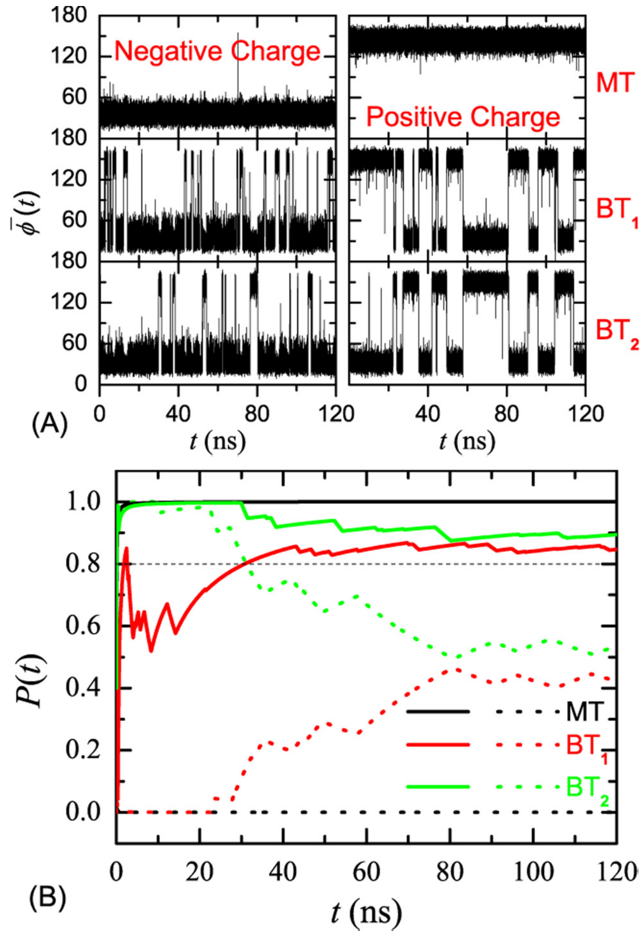
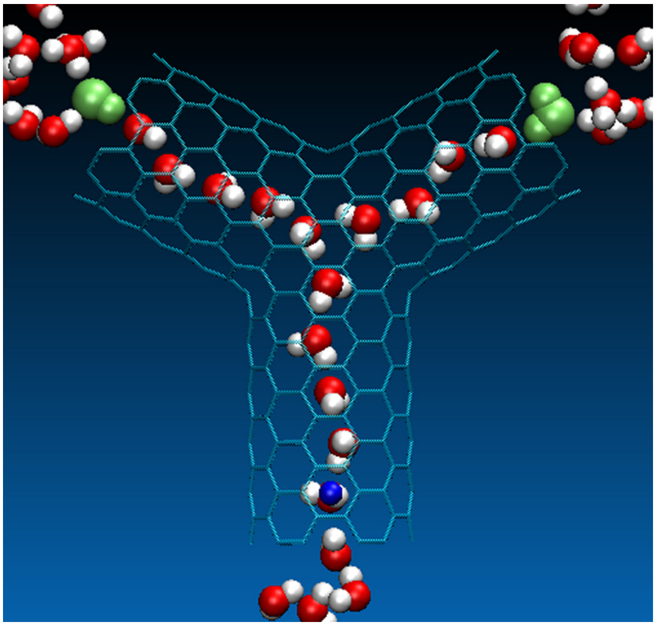
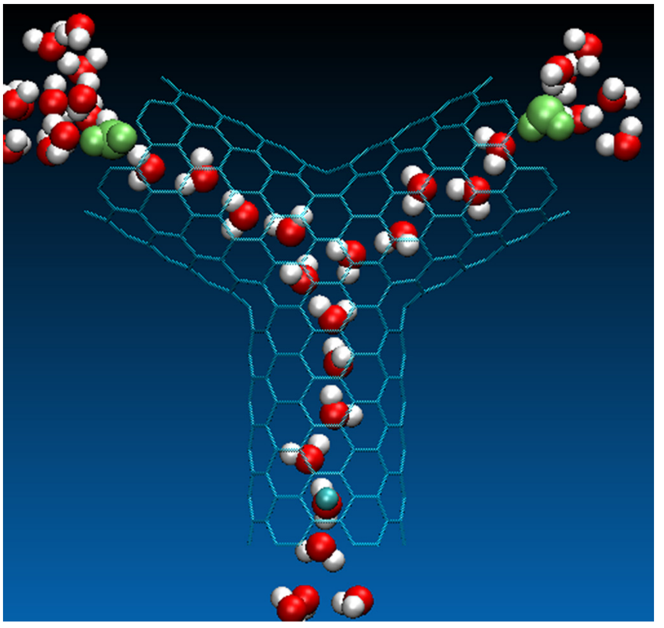


Fig. S3. The average dipole angle $\bar{\phi}(t)$ of the water orientations and the probability of dipole orientation $P(t)$ in each tube for a T-shaped SWNT. (*A*) The $\bar{\phi}(t)$ is shown for a negative charge (*Left*) and a positive charge (*Right*). (*B*) Probability $P(t)$ is shown for a negative charge (solid lines) and a positive charge (dashed lines). Results indicates the same conclusion for the water dipole orientation preferences and water-mediated signal transduction when replacing the 120° angle between 2 branch tubes with a 180° angle (i.e., replacing the Y-shaped SWNT with a T-shaped SWNT).



Movie S1. Videos to show how a negative charge monitors/tunes the concerted dipole orientation distribution of water molecules in the main tube and how this water orientation in the main tube transmit to the water dipole orientation distributions in the two branch tubes. The blue sphere in the videos represents the negative charge. The lime green water molecules are the water molecules just outside the blanch tubes that their dipole orientations are efficiently controlled by the dipole orientations of the water molecules inside the blanch tubes.

Movie S1 (MPG)



Movie S2. Videos to show how positive charge monitors/tunes the concerted dipole orientation distribution of water molecules in the main tube and how this water orientation in the main tube transmit to the water dipole orientation distributions in the two branch tubes. The green sphere in the videos represents the positive charge. The lime green water molecules are the water molecules just outside the blanch tubes that their dipole orientations are efficiently controlled by the dipole orientations of the water molecules inside the blanch tubes.

Movie S2 (MPG)