Supplementary Material

Spontaneous Sieving of Water from Ethanol using Carbon Nanotubes

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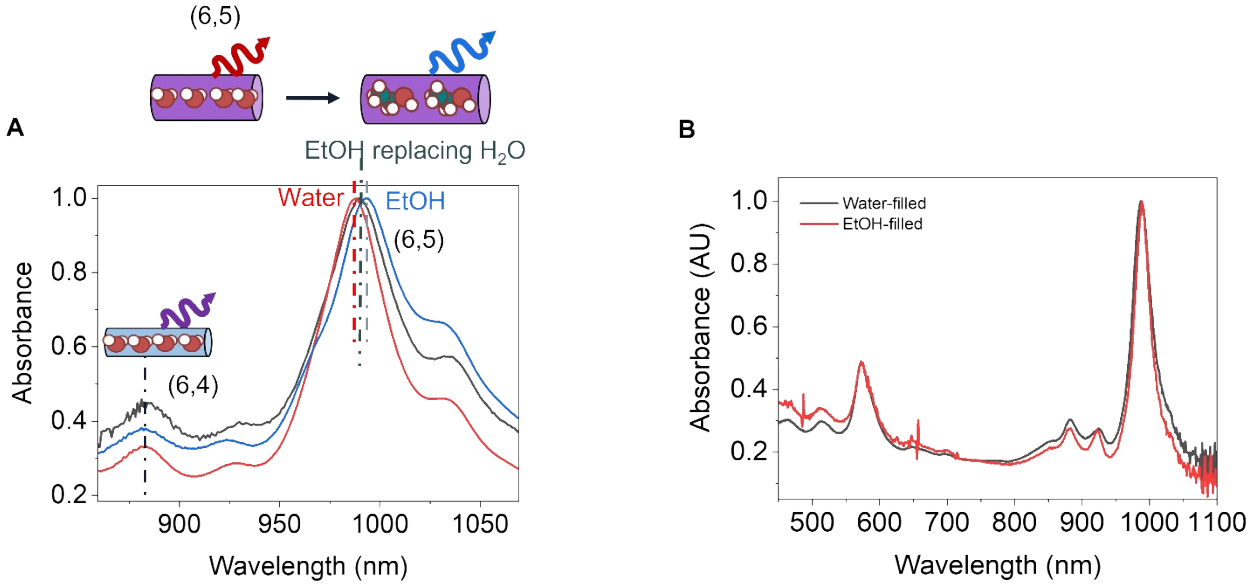
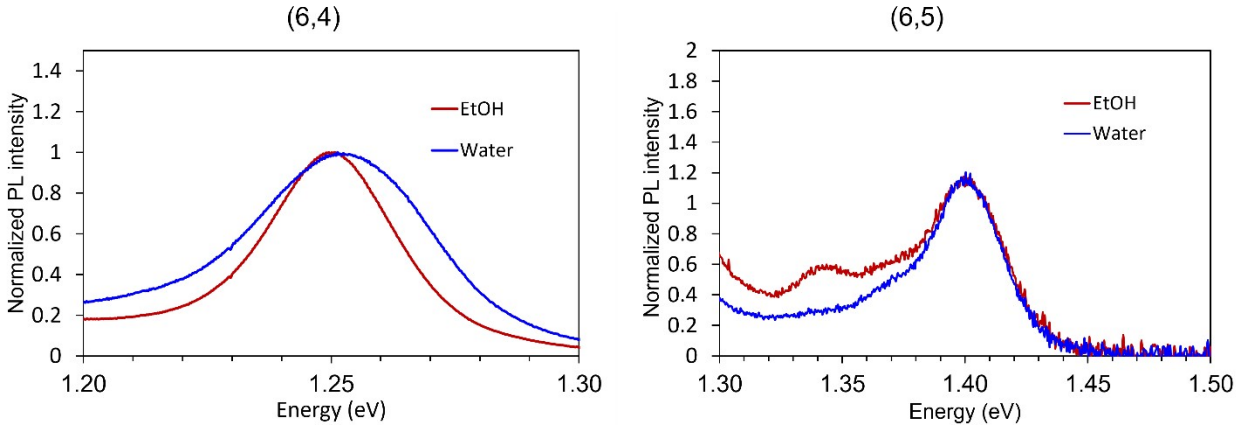
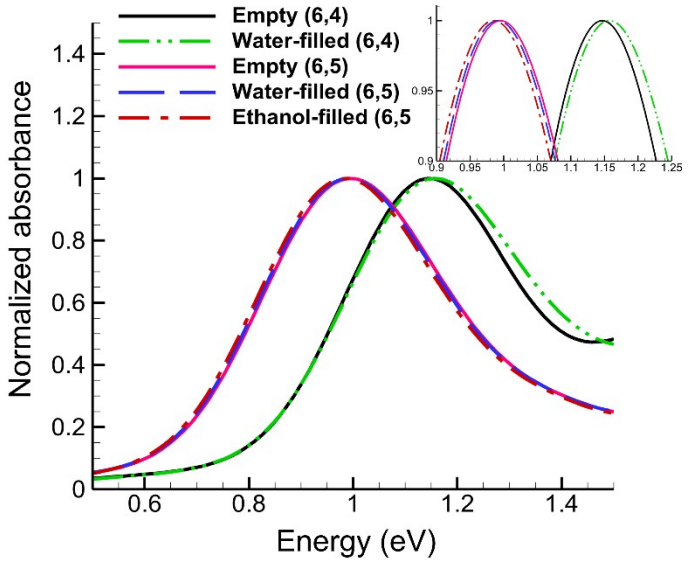


Supplementary Figure 1. Spectroscopic evidence of water-selective filling of small diameter SWCNTs. (**A**) Absorption spectra for (6,4) and (6,5)-SWCNTs that are sequentially incubated in water (red curve)

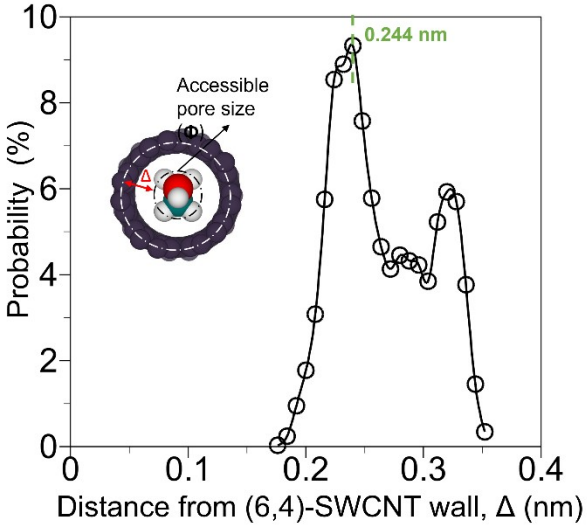
and then in ethanol (blue curve). The green curve shows a transient stage when the water inside the SWCNTs is being replaced by ethanol. For (6,4)-SWCNT, the peak position does not change by ethanol, indicating that water is not replaced by ethanol. For (6,5)-SWCNT, water is replaced by ethanol and is shown by the red and the blue curves, with the green curve being an intermediate state of water-ethanol mixture. A red-shift is observed for (6,5)-SWCNT. (**B**) Full absorption spectra of ethanol and water-filled (6,4), (9,1) and (6,5)-SWCNTs.



Supplementary Figure 2: Photoluminescence (PL) spectra of filling of SWCNTs by water and ethanol from experiments. Initially the (6,4) and (6,5)-SWCNTs are incubated in water and then in ethanol. PL spectra for SWCNTs incubated in water are marked by the blue curve, and those incubated in ethanol afterwards are marked by the red curve. For (6,4)-SWCNT, it is observed that the position of the peak does not change after incubating in ethanol indicating that water is not replaced by ethanol. Similarly, for (6,5)-SWCNT, water is replaced by ethanol and is shown by the blue and red curves and is marked with a red-shift.



Supplementary Figure 3: TD-DFT simulations reveal the origin of the observed spectral shift: The absorption shifts observed through filling of (6,4) and (6,5)-SWCNTs by water and ethanol is plotted, with the insets showing a zoomed in plot near the first absorption peaks. Comparing the shifts, we observe a red-shift in (6,5)-SWCNT as it is filled by ethanol and a blue-shift for water-filled (6,4)-SWCNT compared to the empty SWCNT. The absorption spectra for each of the curves is normalized using the maximum value of the intensity.



Supplementary Figure 4. Distribution of distance from the SWCNT wall (Δ). Probability distribution of the projected radial distance (Δ) between the carbon and hydrogen atoms of the ethanol molecule and the (6,4)-SWCNT wall, used to calculate accessible pore size (Φ) of (6,4)-SWCNT.