Orientation-Driven Water Flow in Nanotubes

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Bidirectional single file water transport in a carbon nanotube is known to occur in “bursts” in short nanotubes. During the last year, we have shown that in long carbon nanotubes, when the orientation of the water molecules is maintained along one direction, a net water transport along that direction can be attained due to coupling between rotational and translational motions. The rotations of the water molecules are correlated more with the translation of the neighboring water molecules with the acceptor oxygen than the neighbor with the donor hydrogen. This mechanism can be used to pump water through nanotubes.

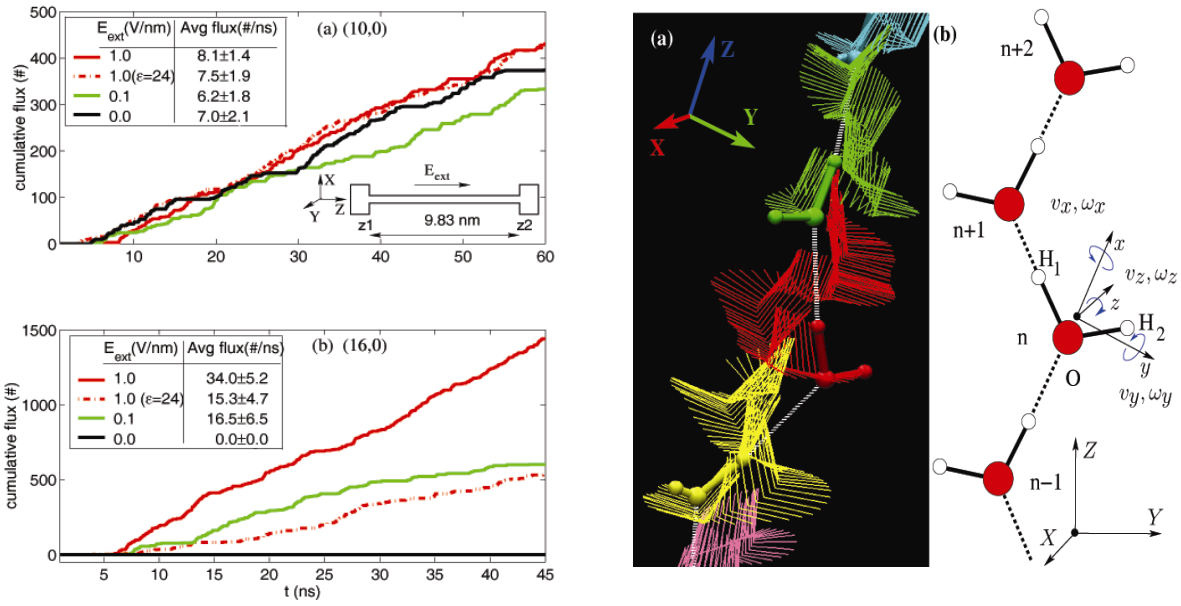

Figure 7.1 shows cumulative flux of water molecules crossing the tube as a function of time for (a) (10, 0) and (b) (16,0) CNTs for various values of *E*ext. (right) (a) Trajectory of water molecules in a (10,0) (*E* = 0 V/nm) CNT. Each color represents a water molecule’s trajectory for 1.9 ps. The ball-stick models (various colors) denote the position of water at *t*=0. (b) Schematic of a single file water with body centered principal axes frame *xyz* and the fixed box reference frame *XYZ*.

S. Joseph and N.R. Aluru, “Pumping of confined water in carbon nanotubes by rotation-translation coupling”, *Physical Review Letters*, Vol. 101, No. 6, Art. No. 064502, 2008.

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