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Rotational-Translational Coupling in Nanopores SONY JOSEPH, N.R. ALURU, University of Illinois at Urbana-Champaign — A rare combination of molecularly smooth walls and hydrophobicity of the surface make carbon nanotube (CNT) membranes fast transporters of water. Though bi-directional single file water transport in "bursts" through a (6,6) CNT and collective intermittent reversing of water dipolar orientations has been observed in molecular dynamics simulation for short tubes, the molecular mechanism governing the relation between the dipole orientation and the flow direction has not been elucidated. Here we show that when the orientation of the water molecules is maintained along one direction in longer tubes, 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 molecule with the acceptor oxygen than the neighbor with the donor hydrogen. By applying an electric field or by attaching chemical functional groups at the tube ends, the orientations can be maintained and this mechanism of rotational-translational coupling can be used to pump confined water through nanotubes.

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