CNT based thermal Brownian motor to pump water in nanodevices

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CNT based thermal Brownian motor to pump water in nanodevices[1] ELTON OYARZUA, HARVEY ZAMBRANO, Universidad de Concepcion, J. H. WALTHER, Technical University of Denmark — Brownian molecular motors are nanoscale machines that exploit thermal fluctuations for directional motion by employing mechanisms such as the Feynman-Smoluchowski ratchet. In this study, using Non Equilibrium Molecular Dynamics, we propose a novel thermal Brownian motor for pumping water through Carbon Nanotubes (CNTs). To achieve this we impose a thermal gradient along the axis of a CNT filled with water and impose, in addition, a spatial asymmetry by fixing specific zones on the CNT in order to modify the vibrational modes of the CNT. We find that the temperature gradient and imposed spatial asymmetry drive the water flow in a preferential direction. We systematically modified the magnitude of the applied thermal gradient and the axial position of the fixed points. The analysis involves measurement of the vibrational modes in the CNTs using a Fast Fourier Transform (FFT) algorithm. We observed water flow in CNTs of 0.94, 1.4 and 2.0 nm in diameter, reaching a maximum velocity of 5 m/s for a thermal gradient of 3.3 K/nm. The proposed thermal motor is capable of delivering a continuous flow throughout a CNT, providing a useful tool for driving liquids in nanofluidic devices by exploiting thermal gradients.

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