

# Characterization of CO<sub>2</sub> flow through charged carbon nanotubes

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## **Abstract**

The equilibrium transport of CO<sub>2</sub> through infinitely long charged and uncharged single-walled carbon nanotubes has been examined by employing molecular dynamics simulations. It has been shown that the molecular transport concludes into a Fickian diffusion for all the examined cases. Ballistic and single-file diffusion mechanisms have been met especially in cases where the degree of loading is low since at higher pressures the electrostatic interactions derived by the charge of the nanotubes is canceled by the stronger SWNT-CO<sub>2</sub> interactions.