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Escape of water molecular from Carbon Nanotubes JIAXI LI, WENFENG LI, JIANWEI ZHANG, Tongji Univ — Understanding and controlling the transport of water molecules through nanopores have attracted great interest due to potential applications for designing novel nanofluidic devices, machines and sensors. In this work, we theoretically investigate the effects of an external nonuniform electric field on the escape of water molecules through single-walled carbon nanotubes (SWNTs) by using of molecular dynamics (MD) simulations. When polar water molecules are placed in the gradient electric field, the electric force is experienced that can drive the water molecules. Molecular dynamics simulations show that the escape probability of water obeys the Boltzmann distribution. Our results show that energy barrier delta E is independent of temperature which indicates that it is a single-barrier system. From the MD results statistics, the key parameters could be determined such that the relationship between energy barrier delta E and diameter of SWNTs and nozzle distance of the charge r would be revealed that could deepen our current theoretical understanding on transport of water molecular inside SWNTs with the nonuniform electric field.

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