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**Frictional energy barrier and blocking temperature in water molecules and carbon nanotubes system**<sup>1</sup> JIANWEI ZHANG, JIAXI LI, WENFENG LI, School of physics, Tongji University — Water transport through hydrophobic channels of single-walled carbon nanotubes has attracted a lot interests, especially, various potential applications of SWCNTs have been proposed for designing novel nanofluidic devices. By adopting Molecular dynamics method, we investigated mechanics and statistics properties of water molecules escaping from a confined single-walled carbon nanotube. From our numerical MD simulations and statistical model, we determined the friction energy barrier of water molecules in (10,10) SWCNT is 9.88 kcal/mol, and which is the minimal energy for flowing a water molecules in CNT. By only using friction energy barrier and relaxation time parameter, our model can fit all different situations MD simulation results. In order to describing the frictional lock behavior of water molecules, we introduced a new blocking temperature, below this temperature (391K for our system), water is locked in CNT due to friction energy barrier. We found that the blocking temperature is closely related to system response time, and it also shows a linear behavior to frictional energy barrier. Furthermore, we found several other interesting statistics results when a water molecules leaving SWCNTs.

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Jianwei Zhang  
School of physics, Tongji University

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