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Research paper

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Min Zhou, Ying Hu, Jian-chuan Liu, Ke Cheng, Guo-zhu Jia

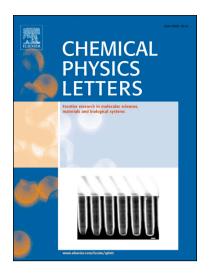
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Hydrogen Bonding and Transportation Properties of Water Confined in the Single-walled Carbon Nanotube in the Pulse-Field

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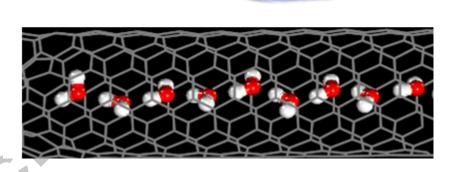
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Z-direction



Highlights:

Time-varying pulse-field hinders the movement of water in SWCNT.

The hydrogen bonding lifetimes depend on the frequency of pulse-field.

Abstract

In this paper, molecular dynamics simulations were performed to investigate the transportation and hydrogen bonding dynamics of water confined in (6, 6) single-walled carbon nanotube (SWCNT) in the absence and presence of time-dependent pulse-field. The effects of pulse-field range from microwave to ultraviolet frequency on the diffusivity and hydrogen bonding of confined water were

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