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受限于不同螺旋性的纳米碳管中水的分子动力学模拟

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摘要 近年来将纳米碱米碳管引入到与生命过程息息相关的离子通道膜的研究逐渐成 为热点，
而其中的关键就是要了解受限于膜孔道（碳管）中水分子的行为。采用分 子动力学模拟在300 K和1.01 * 10~5 Pa下对受限于（6，6）armchair型和（10， 0）zigzag型纳米碳管中的水进行了研究，
得到了水分子在碳管中的局部密度分布 等静态性质以及水分子在碳管中的传递等动态性质，
并对不同势能模型的模拟结果 作了比较。结果表明选择不同的势能模型并没有改变此体系的固有性质，
即水分子 不仅能够进入到憎水性的（6，6）碳管中而且能形成一条稳定的由氢键相连的纵列 （single file），
而且在管中以纵列的形式进行同歇传递。此外，碳管螺旋性对
受限水的静态性质影响不大但对动态性质则有一定程度的影响，水分子在（10，0 ）
zigzag型碳管中的传递能力要强于在（6，6）armchair型碳管中的能力。

关键词 碳 纳米相材料 水 动力学

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Molecular Dynamics Study of Water Molecules Confined in Carbon Nanotubes with Different Helicity

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Abstract Recently one promising area of studying nanotubes involves modeling them to mimic real ion channels in biological systems, which may greatly reduce the complexity of modeling ion channels. However, this can only be possible with a comprehensive understanding of the interactions of ion channels (nanotubes) with water molecules. In addition, the properties of a nanolube strongly depend on its helicity, therefore the effect of helicity on behaviors of water molecules confined in nanotubes deserves further investigation. The behaviors of water molecules confined in (6, 6) armchair and (10,0) zigzag type lubes were analyzed by molecular dynamics simulation at 300 K and 1.01 * 10~5 Pa. Static properties including water density profiles inside tubes and dynamic properties such as water transport through tubes were obtained. The effect of potential models on the simulation results was compared. The results indicate that the innate chaiticteristics of such system do not depend on different potential models. Water molecules can flow into hydrophobia carbon lubes to form a stable hydrogen-bonded chain called single file, and spontaneously conduct through tubes as the single file form. Helicity rarely affects static properties of water molecules confined in nanotubes but does influence dynamic properties to some extent. The ability of water conduction through (10,0) zigzag type tube is stronger than that through (6,6) armchair type tube.

Key words CARBON NANOPHASE MATERIALS WATER DYNAMICS

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