عنوان مقاله:

Calculation of water molecules properties in the single wall carbon nanotube

محل انتشار:

ششمین کنگره بین المللی مهندسی شیمی (سال: 1388)

تعداد صفحات اصل مقاله: 5

نویسنده:

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خلاصه مقاله:

Mathematical modeling of the flow of fluids, and in particular of water, through carbon nanotubes has increasingly attracted the interest of researchers in the last years. Here we reported some properties of water molecules in the single wall carbon nanotube (SWCNT) such as axial and radial density, hydrogen bonding and potential energy of water molecules by performing molecular dynamics simulations (MDS). The results were compared with the properties of water molecules in the bulk. These results have good agreements with other research results so this .method would be a reasonable way for analyses of properties of fluid such as water in the nanoscale materials

کلمات کلیدی:

molecular dynamics simulation (MDS), Carbon nanotube (CNT), hydrogen bonding, radial density