









The nano-pumping process of C_{20} molecules from carbon nanotube at the different external electric fields and atomic defects: A molecular dynamics approach

Haichun Niu ^a, , , Rassol H. Rasheed ^b, S. Mohammad Sajadi ^c, Dheyaa J. Jasim ^d, Soheil Salahshour ^{e, f, g}, Navid Nasajpour-Esfahani ^h, Rozbeh Sabetvand ⁱ, , 

Show more 

+ Add to Mendeley  Share  Cite

<https://doi.org/10.1016/j.diamond.2023.110735>

[Get rights and content](#) 

Abstract

Today, carbon nanotubes are involved in many medical types of research, such as biosensors and drug delivery. These nanotubes do not pose a problem for the body regarding toxicity to body cells and triggering the immune system. Nanotubes have also been proven to increase solubility and the possibility of targeted drug delivery. This study used molecular dynamics simulation to examine the nano-pumping process of the C_{20} molecule in carbon nanotubes at the different electric fields and atomic defects. The process of C_{20} molecule nano-pumping was examined by examining the changes in kinetic energy, potential energy, entropy, stress, temperature, and internal energy changes. In the following, the stress on the atomic structure was calculated. For this purpose, constant electric fields with the magnitudes of 0.01, 0.02, 0.03, 0.05, and 0.1 V/Å are used for the atomic structure. The results show that the nano-pumping time of the C_{20} molecule in the carbon nanotubes increases by increasing the electric field magnitude. The results also revealed that the kinetic energy in the structure decreased by increasing the electric fields, and the potential energy increased. As the potential energy increased in the atomic structure, the stability increased. Therefore, it is expected that the C_{20} molecule nano-pumping time will increase. The following examined the effect of atomic defects in an electric field with a magnitude of 0.01 V/Å. For this purpose, the atomic defects with magnitudes of 1%, 2%, 3%, and 4% were used for carbon nanotubes. The results revealed that increasing the atomic defects increased the C_{20} molecule nano-pumping time. Furthermore, the stress on the structure increased by increasing the atomic defects.