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Variable electric field and atomic percentage of doping on the displacement process of C_{20} molecules in a nanotube with molecular dynamics simulation

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Abstract

The displacement of the C20 molecule in the presence of different electric field frequencies (EFFs) and silicon (Si) doping on the carbon nanotube (CNT) was examined in this work using the molecular dynamics (MD) method. Time variable EFs with various frequencies and magnitudes of 0.1, 0.2, 0.4, and 0.6THz were applied to the CNT to study the effects of an EF. The C20 molecule moved at a faster rate as a consequence of an increase in the EEF, which increased the structure's kinetic energy (KE). The KE parameter reached 5.01eV using EFF with 0.6THz magnitudes. So, increasing EFF caused translational displacement of the target molecule, and the nano-pumping process was done in a shorter MD time (7.15 ps). Moreover, the lattice stress on fullerene increased from 4.23×106bar to 8.84×106 by increasing the EFF to 0.6THzeV after 8 ps. This atomic performance arose from more resistance of atomic nanotubes in target molecule displacement. Considering the nano-pumping process of C20 molecule in the presence of an EFF with a magnitude of 0.6THzeV performed better than other atomic samples, the effect of Si doping on the nano-pumping process in this EF was studied. So, Si particles with atomic percentages of 0.01, 0.02, and 0.05 were added to CNT. The results reveal that the displacement time of C_{20} molecules increased by increasing atomic percentage of Si doping. In the presence of a 5% atomic percentage of Si doping, the displacement time of the C20 molecules increased from 7.73 to 8.08 ps.