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Structural and elastic properties and stability characteristics of oxygenated carbon nanotubes under physical adsorption of polymers

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Abstract: The importance of covalent and non-covalent functionalization approaches for modification the properties of carbon nanotubes is being more widely recognized. To this end, elastic properties and buckling behavior of oxygenated CNT with atomic oxygen and hydroxyl under physical adsorption of PE (Polyethylene) and PEO (Poly (ethylene oxide)) are determined through employing the molecular dynamics (MD) simulations. The results demonstrate that non-covalent bonding of polymer on the surface of oxygenated CNT causes reductions in the variations of critical buckling load and critical strain compared to oxygenated CNTs. Critical buckling load and critical strain of oxygenated CNT/polymer are higher than those of oxygenated CNT. Also, it is demonstrated that critical buckling load and critical strain values in the case of oxygenated CNT/polymer are independent of polymer type unlike the value of Young's modulus. It is shown that variations of Young's modulus decrease as PE adsorbed on the surface of oxygenated CNT. Moreover, the presence of oxygen atom on PEO chain leads to bigger variations of Young's modulus with weight percentage of chemisorbed component, i.e. atomic oxygen and hydroxyl. It is also demonstrated that Young's modulus reduces more considerably in the presence of PEO chain compared to PE one.

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