Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information

A Coarse Grained Molecular Dynamics Simulation Study on the Structural Properties of Carbonnanotube-Dendrimer

Sajjad Kavyani[a], Mitra Dadvar[a], Hamid Modarress[a†], Sepideh Amjad-Iranagh[a]

[a] Department of Chemical Engineering, Amirkabir University of Technology

[*] Corresponding Author

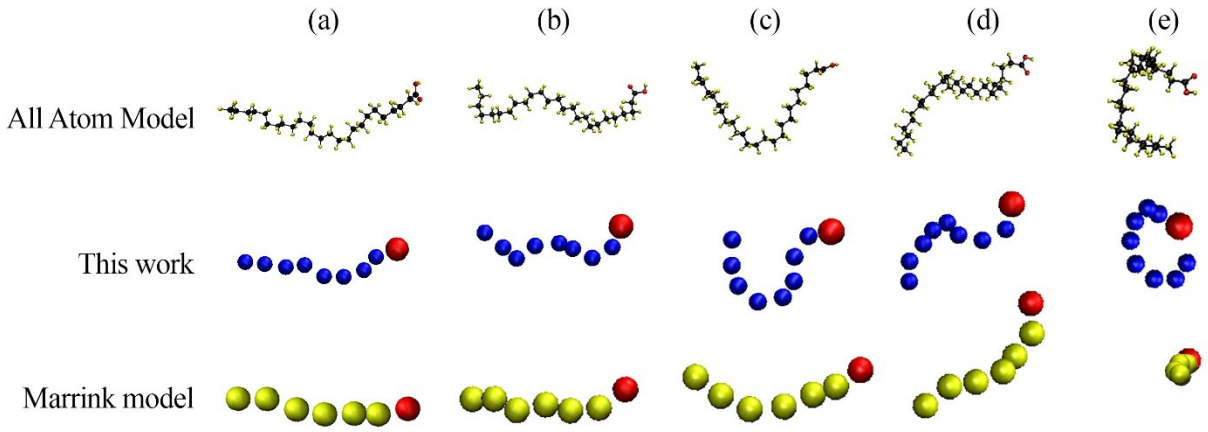

Figure S1. Randomly chosen structural conformations of FTA molecule ($C_{25}H_{50}O_2$) in the course of simulations including: all atom, this work and Marrink model. (a to d) Folding and (e) Torsion.

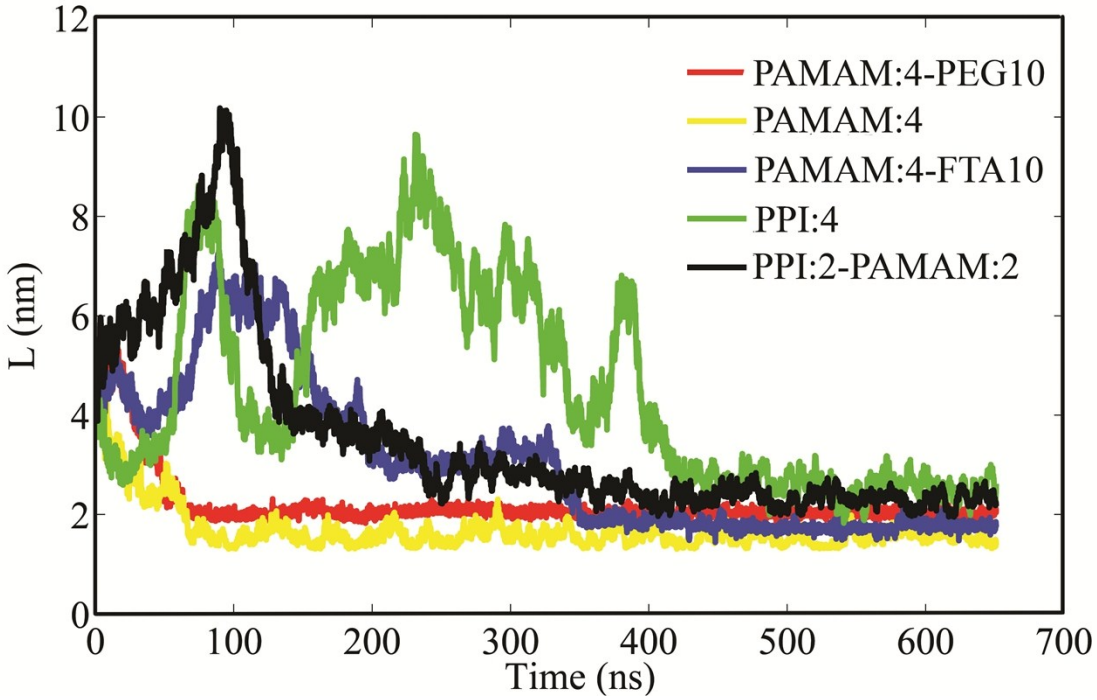

Figure S2. Distance (L) between centre of mass (COM) of dendrimer complexes and CNT versus time for some randomly selected CNT-dendrimer complexes