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Molecular Dynamics of Fatty Acid Interacting with Carbon Nanotube as Selective Device

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***Abstract*—**In this paper we study a system composed by carbon nanotube (CNT) and bundle of carbon nanotube (BuCNT) interacting with a specific fatty acid as molecular probe. Full system is represented by open nanotube (or nanotubes) and the linoleic acid (LA) relaxing due the interaction with CNT and BuCNT. The LA has in his form an asymmetric shape with COOH termination provoking a close BuCNT interaction mainly by van der Waals force field. The simulations were performed by classical molecular dynamics with standard parameterizations.

Our results show that these BuCNT and CNT are dynamically stable and it shows a preferential interaction position with LA resulting in three features: (i) when the LA is interacting with CNT and BuCNT (including both termination, CH2 or COOH), the LA is repelled; (ii) when the LA terminated with CH2 is closer to open extremity of BuCNT, the LA is also repelled by the interaction between them; and (iii) when the LA terminated with COOH is closer to open extremity of BuCNT, the LA is encapsulated by the BuCNT. These simulations are part of a more extensive work on searching efficient selective molecular devices and could be useful to reach this goal.

***Keywords*—**Carbon Nanotube, Linoleic Acid, Molecular Dynamics.

I. Introduction

INTRINSIC selectivity devices appear in nature in several forms as, for instance, in biological systems when ionic channels are opened or closed in specific conditions as pH, temperature among others [1]. Within new technological advances have preclude to necessity of design selective devices [2]. An effort has been made to create devices with high selectivity beyond our present micromachining[3, 4].

Tian et al. have described the synthesis, characterization and self-assembly of a modified linoleic acid + polypeptide presenting with drug release behavior prepared by ring-opening polymerization. They found by aggregation concentration assessed by fluorescence measurement that it could be employed as molecular probe [5]. Molecular dynamics simulations performed using carbon nanotube including constriction show that entropic effect can be dominant when interacting with molecules with similar sizes concluding that it could useful for permeation selectivity [6]. Also, dispersion of linoleic acid has been used as fluid to stabilize nanoparticles and nanotubes showing direct evidence of viscosity of the dispersion could change depending on the loading fraction of carbon nanotubes showing that viscosity increases by up to 60% and this increase will vary depending on the type of oil system used [7].

In this work, we have simulated by classical molecular dynamics with state-of-art molecular force field [8, 9] including bond angle bend, bond stretch, diedral rotation, and van der Waals terms for one carbon nanotube (CNT) and a bundle of carbon nanotubes (BuCNT) interacting with linoleic acid (LA) working as molecular probe and representing two possibilities of interaction between the systems as: LA with head and tail in opposite directions to reach the CNT and BuCNT. Also, for CNT were investigated two sizes as CNT(10,10) and CNT(8,0). In top panel of Figures 1, 2, 3, 4, and 5 are a picture of these simulations.

II. Methodology

This methodological feature has been guarantied to be very effective in the investigation of dynamic signature of CHON (carbon, hydrogen, oxygen, and nitrogen) structures [9, 10, 11, 12, 13, 14]. The convergence criteria for all calculations were based on previous works done and tested by us [11, 12, 13] as: The energy differences, maximum force, and maximum atomic displacement equal to 10^{-4} kcal/mol, 10^{-3} kcal/mol/Å, and 10^{-5} Å, respectively. Also, the root mean square deviations and displacement as 10^{-3} kcal/mol/Å and 10^{-5} Å, respectively. After minimization procedures selective canonical dynamics was permitted with time steps of 1 fs were accomplished for all calculations.

The generation of structures were followed by carbon nanotube (CNT) open at both extremities acting as a shell barrier and confronted with linoleic acid surrounded. Both carbon nanotubes ((10,10) and (8,0)) that forms the device were separately optimized (including standards grounds for energy and geometry) and reoptimized when put them interacting. After that we attribute several initial position for LA (as previous described) in order to initialize the full simulation.

III. Results and Discussions

In Figure 1(middle), it is presented the simulation of molecular dynamics to the case where the LA has the CH_2 group interacting with the CNT. The potential and kinetic energies have a flotation due the interaction among the atoms of LA + CNT. These energies show *in*-phase mode producing the same dynamical signature. The net effect of LA over the CNT can be seen as an oscillatory period of 10 ps. Corroborating this feature, we plot out the non-bond energy showing very low variation illustrated as background

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flotation. Also, Figure 1(bottom) shows the temperature behavior, and it can be described as a simple model of considering the motion of the center-of-mass due repulsion of the van der Waals forces that acting on. Complementary video presented in references [14, 15] show the dynamic evolution.

Also in opposite configuration LA (Figure 2 where *COOH* group closer to CNT) and the net effect are the same remaining oscillatory frequencies due the repulsive force as signature of dynamic properties. For small CNT as (8,0) presented in Figure 3, the results presents almost no fluctuation and oscillatory period of 6 ps.

For the BuCNT (Figures 4 and 5), the results demonstrated that this repulsion effect can disappear due the interactions between the nanotubes and LA inducing massive transfer momentum between them affecting the oscillatory behavior and it could be see in Figure 5. Figure 5 shows the energies presenting no sustained oscillatory regime and huge flotation provoking the non-bonded energy playing important rule changing the signal as typical behavior of exchange interaction between LA and BuCNT. The capture of LA inside a specific nanotube show oscillatory regime representing shelled and stable LA + BuCNT. The same oscillatory regime is followed for temperature. See complementary videos presented in references [14, 15].

It raises an important question how to apply these findings to work as selective molecular device in a controllable way. An insight could be by applying external electric or magnetic fields in the fatty acid to align in a preferential direction. Also, it is possible to separate selectively BuCNT with/without fatty acid.

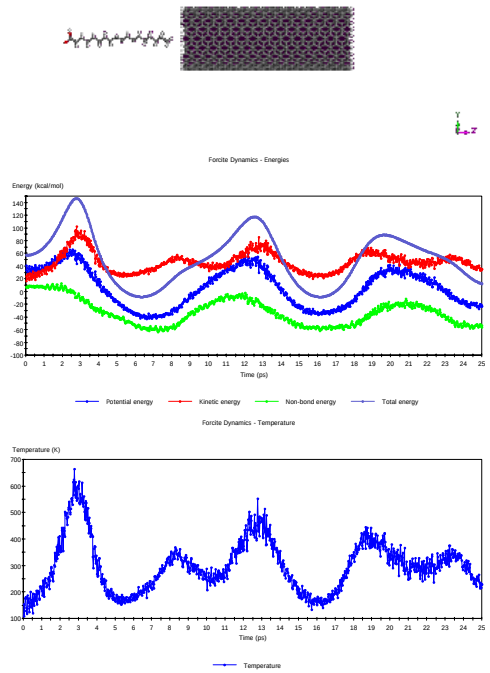

Fig. 1 Pictogram representation of the proposed linoleic acid and carbon nanotube (10,10) where (*top*) CH_2 molecular termination was simulated. (middle) Total, potential, kinetic, and non-bonded energies, as well (bottom) temperature results from molecular dynamics simulations. These results refer to the case where LA is captured by the CNT(10,10) showing dissipative effects up to 15 ps. The LA total energy shows fluctuation due interaction with CNT.

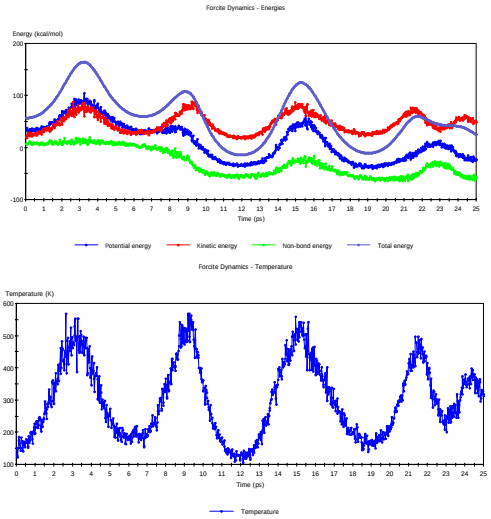

Fig. 2 Linoleic acid and carbon nanotube (10,10) where *COOH* molecular termination was simulated. (*top*) Total, potential, kinetic, and non-bonded energies, as well (bottom) temperature results from molecular dynamics simulations. Also the results refer to the case where LA is captured by the CNT(10,10) showing a larger repulsion due van der walls effects (up to 9 ps) when compared with CH_2 termination.

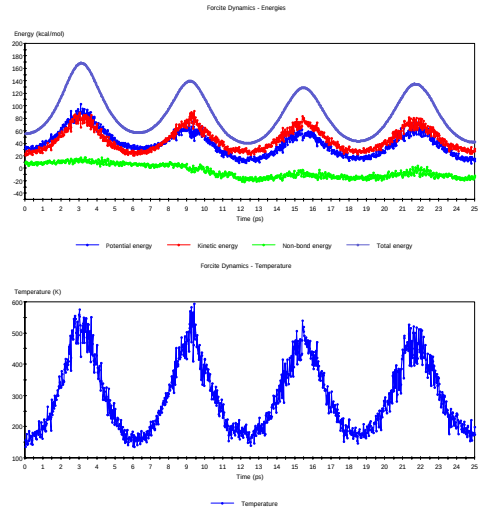

Fig. 3 Typical total, potential, kinetic, and non-bonded energies, as well (bottom) temperature results from molecular dynamics simulations. These results refer to the case where LA is not captured by the CNT(8,0) showing no dissipative effects with very small fluctuation due the interaction between them.

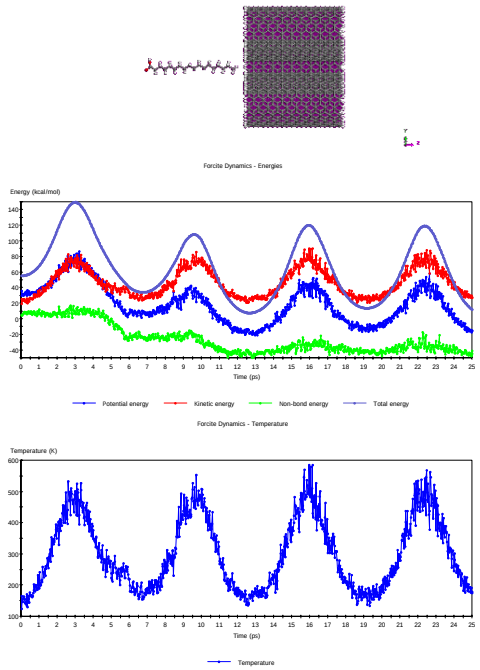

Fig. 4 (*top*) Pictogram representation of the proposed linoleic acid and bundle of carbon nanotube (10,10) where CH_2 molecular termination was simulated. (*bottom*) Total, potential, kinetic, and non-bonded energies from molecular dynamics simulations. (*bottom*) Temperature effect. The results presented here refer to the case where LA is not captured by the BuCNT showing no dissipative effects with very small fluctuation due the interaction between them.

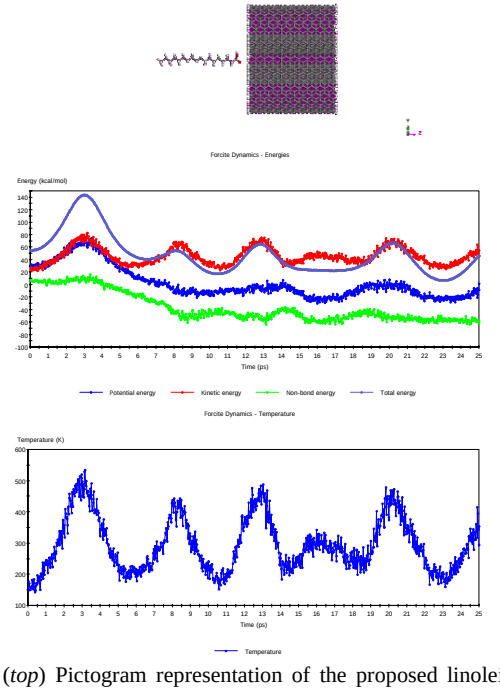

Fig. 5 (*top*) Pictogram representation of the proposed linoleic acid and bundle of carbon nanotube (10,10) where *COOH* molecular termination was simulated. (*middle*) Total, potential, kinetic, and non-bonded energies, as well (b) temperature results from molecular dynamics simulations. The results refer to the case where the BuCNT encapsulated the LA. It shows dissipative effects in energies and temperature when the interaction between both systems (LA + BuCNT) becomes strong.

IV. Summary and Conclusions

This selective molecular device could work with specific experimental parametrization, and to avoid residual contamination it is important to rise up the differences between ideal and real system in the dynamic signature.

We can summary our results as: *(a)* Energies (kinetic, and potential) are in phase and directly proportional to the temperature when repulsive action is more favorable (LA with CH_2 or *COOH* group interacting with the CNT and LA with CH_2 + BuCNT). *(b)* Only the potential energy is in-phase and directly proportional to the temperature when attractive action is the main one (LA with *COOH* group interacting with the BuCNT). After that (LA encapsulated by BuCNT), the all system are stabilized showing the same qualitative feature as (i).

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[15] The files cnt10-10-alin-C.avi, cnt10-10-alin-O.avi, cnt8-0-alin-C.avi, cnt8-0-alin-O.avi, bun10-10-alin-C.avi, bun10-10-alin-O.avi, are the simulations presented in Figure 1, 2, 3(left), 3(right), 4, and 5, respectively.