Molecular dynamics of POPC and POPE lipid membrane bilayers enforced by an intercalated single-wall carbon nanotube

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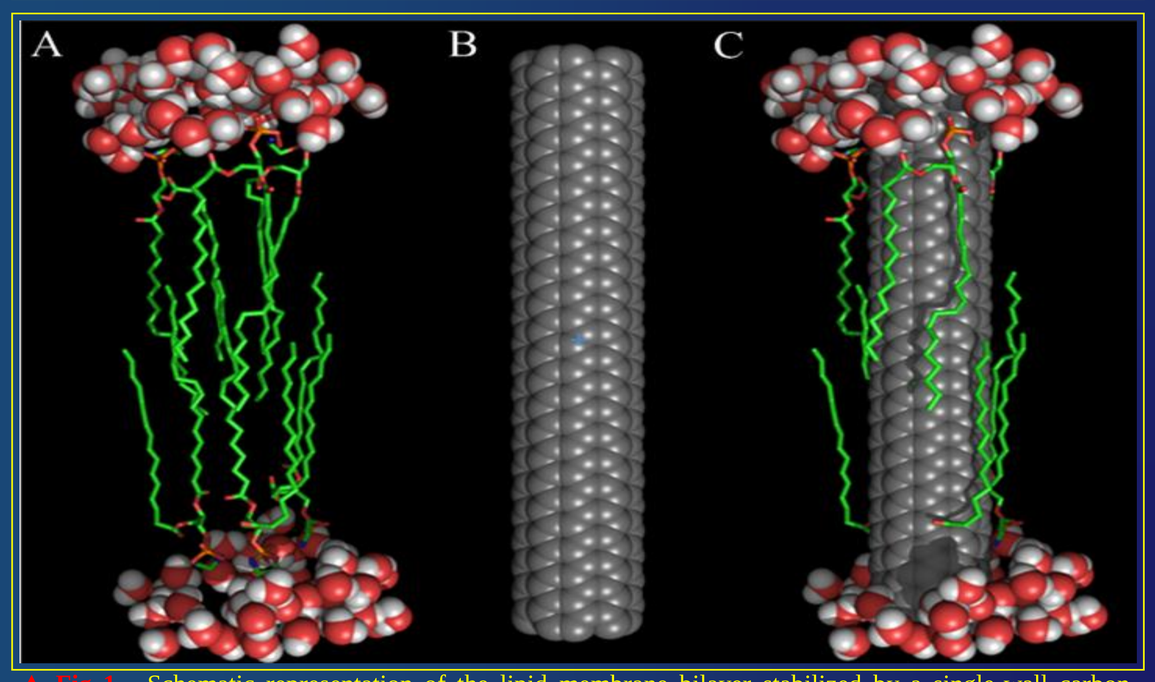
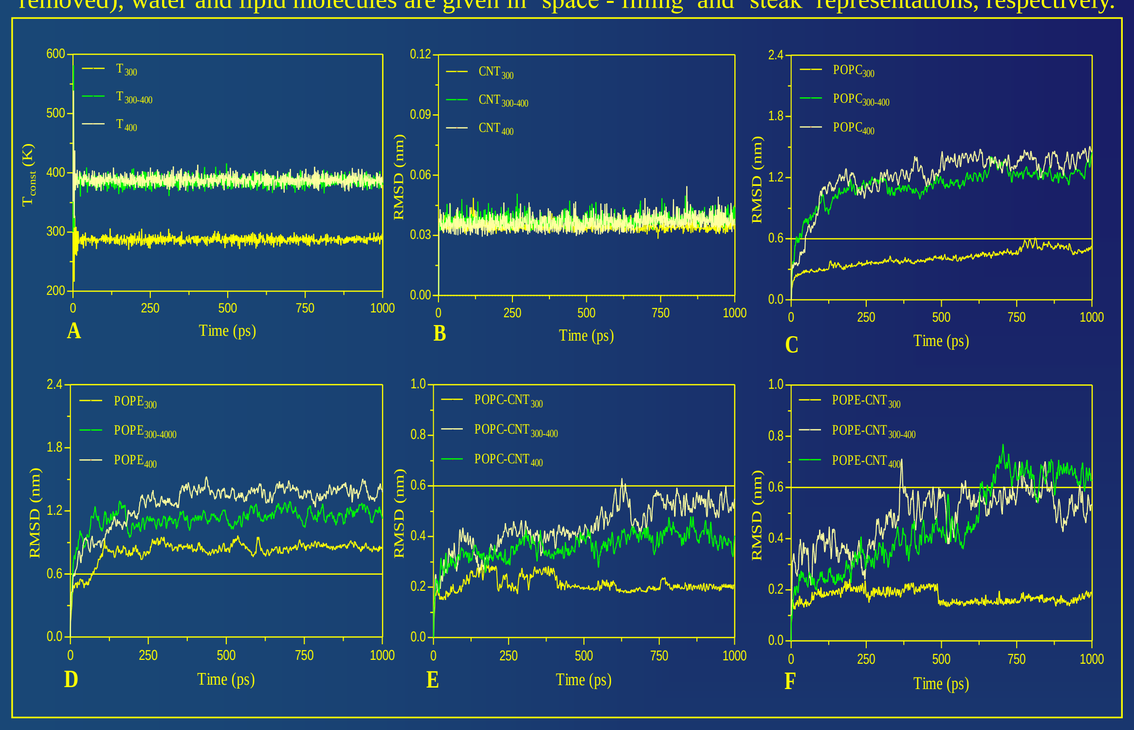
ABSTRACT

The importance of nanotechnology for biotechnological applications is frequently discussed in the scientific community as a powerful tool for the development of nanostructured materials. These nanomaterials support and stabilize biological systems such as lipid bilayer membranes **[1]** and presumably their transmembrane proteins. Black membranes may self-organize from bilayer-forming phospholipids, which are quite stable at room temperature **[2].** It was recently shown that palmitoyl-oleoyl-phosphatidylcholine (POPC) membrane bilayer was supported by hydrophobic carbon nanotube (CNT) network to create mechanically strong surface and increase structural stability **[3].**

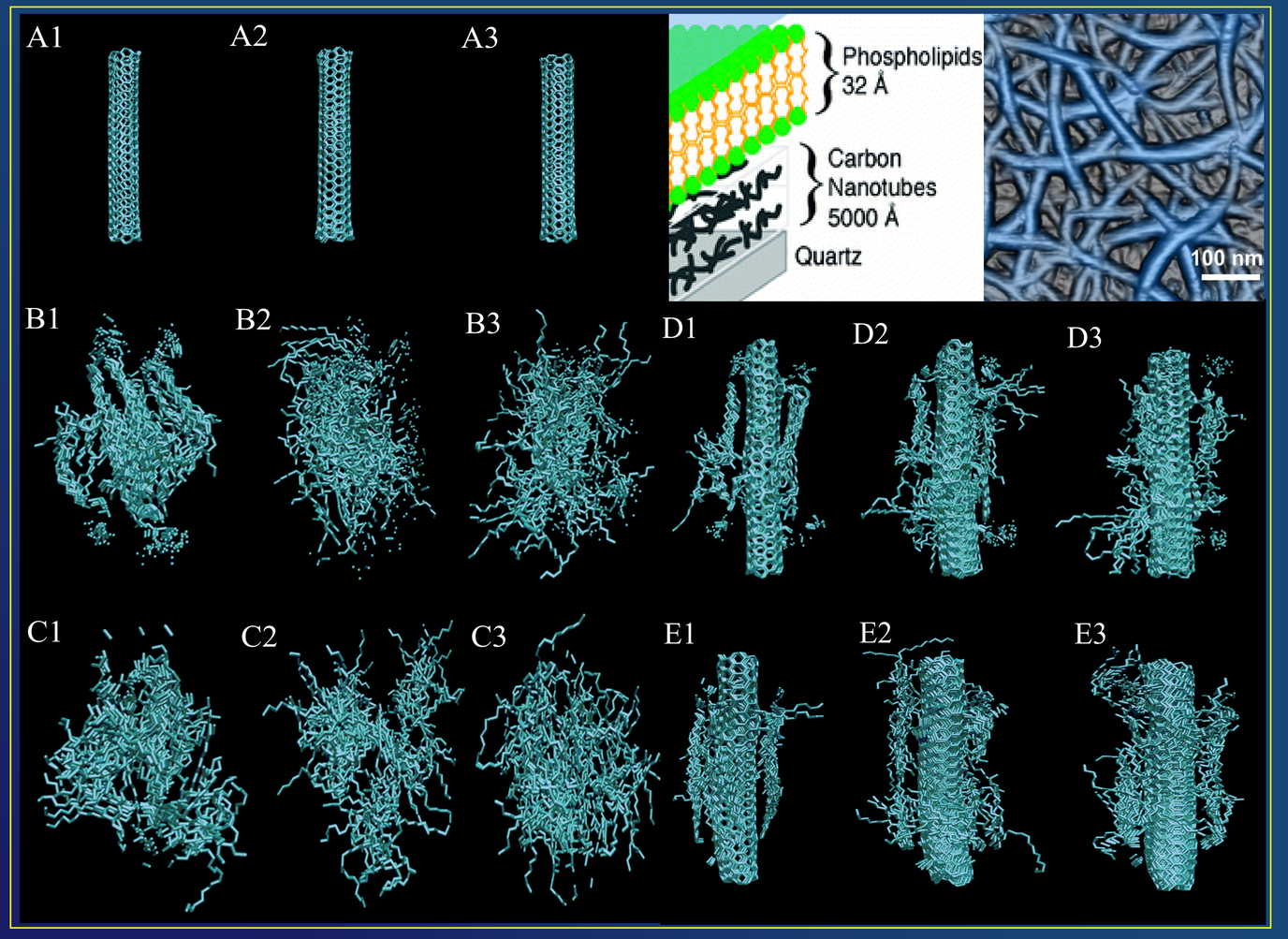
Unfortunately, lipid membranes are very fragile and their stability is difficult to characterize using conventional *in vitro* and *in vivo* methods. However, *in silico* theoretical methods have been used in recent years to tackle this issue. In this study, we used high temperature molecular dynamics simulation (400 K), because it is known that critical fluctuations of lipid membranes can even occur at 313 K and especially above 343 K the interlamellar water layer thickness starts to increase non-linearly due to "hydration force"**[4].** We implemented this method to emphasize POPC and POPE (palmitoyl-oleoyl-phosphatidylethanolamine) membrane bilayer stability enhanced with single-wall carbon nanotube.



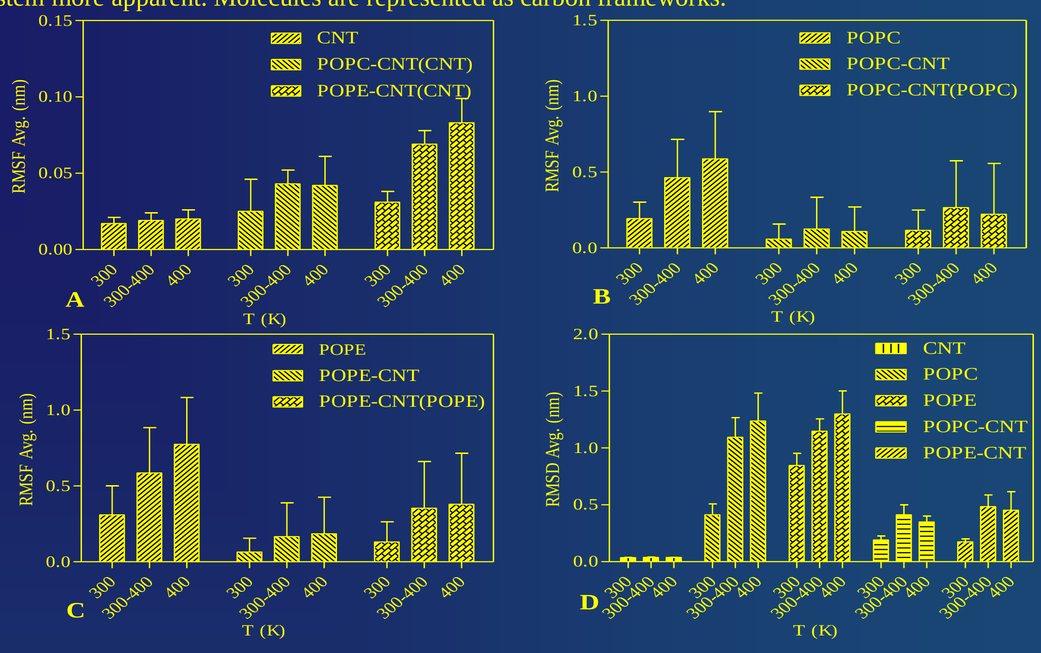
▲ Fig 1 - Schematic representation of the lipid membrane bilayer stabilized by a single-wall carbon nanotube: **(A)** Lipid membrane; **(B)** CNT structure; **(C)** Membrane-CNT complex. CNT (hydrogen atoms removed), water and lipid molecules are given in 'space - filling' and 'steak' representations, respectively.



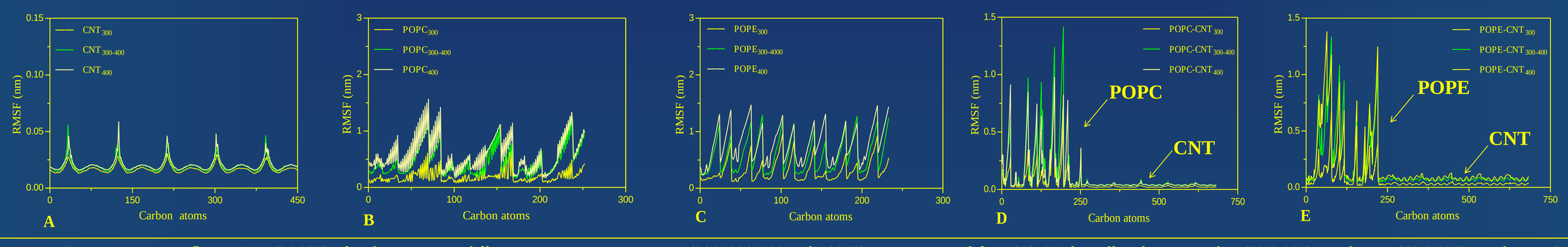
◄ Fig 2 - **(A)** Constant temperature parameters and **(B-F)** RMSD values are shown during 1000 ps evolution time. All RMSD values of investigated MD systems are represented with respect to their initially minimized structures at different temperature levels.



▲ Fig 3 – Visualization of the molecular dynamics trajectories (multiple frames) at different temperature parameters (300, 300-400 and 400 K): **(A1-A3)** Single-wall carbon nanotube; **(B1-B3)** POPC membrane; **(C1-C3)** POPE membrane**; (D1-D3)** POPC-CNT complex**; (E1-E3)** POPE-CNT complex. Images of every hundredth frame are shown simultaneously to make the large-scale motion of the system more apparent. Molecules are represented as carbon frameworks.



▲ Fig 4 – Comparative characteristics of the average root mean square fluctuation and deviation (RMSF, RMSD) values of different simulated structures and substructures at different temperature parameters (300, 300-400 and 400 K): **(A)** RMSF average values of 'native' CNT system and the CNT substructures from different membrane-CNT systems; **(B)** RMSF average values of 'native' POPC, POPC-CNT systems and POPC substructure; **(C)** RMSF average values of 'native' POPE, POPE-CNT systems and POPE substructure. All substructural average RMSFs and RMSDs **(D)** were calculated with respect to initial RMSF values of represented substructures, extracted from the corresponding dynamically simulated systems.



▲ Fig 5 - Root mean square fluctuations (RMSF) of carbon atoms at different temperature parameters (300, 300-400 and 400 K) are represented for: **(A)** Single-wall carbon nanotube; **(B)** POPC membrane; **(C)** POPE membrane**; (D)** POPC-CNT complex**; (E)** POPE-CNT complex during molecular dynamics simulation. The periodic pattern shows the position of carbon atoms in CNT structure as sharp peaks interspaced by low fluctuating atoms. The calculated RMS fluctuations (fluctuations of the water molecules are not shown) show that amplitude is minimal at the ends of the nanotube. The peaks of increased flexibility are represented in the nanotube 'body' due to the low binding frequency motion of the CNT. Peaks at identical position relate to the corresponding atoms in different models. Atom numbering is from one end of the CNT to another.

CONCLUSION

We have shown that CNT intercalation to the lipid membrane elicits remarkable transformation in the structural organization of planar membrane architecture via increasing its dynamic stability. The results derived from this work may be of importance in developing stable nanobiodevices for delivery of various biomolecules in fields of biosensors, biomatherials and biophysics.

REFERENCES

[1] X. Zhou *et al., Nat. Nanotechnol.*, 2(3): 185-190 (2007) [PMID: 18654251] , **[2]** J. Stern *et al., Biochim Biophys Acta.*, 1128(2-3):227-36 (1992) [PMID: 1420295], **[3]** J. Gagner *et al., Langmuir.*, 22(26):10909-11 (2007) [PMID: 17154562], **[4]** S. Kirchner *et al., Europhys. Lett.*, 23 229-235 (1993)