Carbon Allotrope Nanotubes for CO_2 Adsorptions

B. A. Chavez Santos, J. Gomez Quispe, C. Rojas Ayala

Universidad Nacional Mayor de San Marcos, Federal University of ABC. **Email: brandon.chavez@unmsm.edu.pe**

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1. Introduction

This study examines the potential of carbon nanotubes derived from emerging carbon allotropes containing non-hexagonal rings, including Tolanene- and Pha-graphene–based nanotubes, as candidates for CO_2 capture [1,2]. In contrast to conventional CNTs dominated by hexagonal networks, these architectures incorporate unconventional ring topologies that modify local curvature, surface corrugation, and the distribution of adsorption sites, which can directly impact gas–surface interactions. Using reactive molecular dynamics simulations (ReaxFF), we quantify the time-dependent CO2 uptake at 100, 300, and 500 K and compare adsorption stability across nanotube types. The results allow us to establish clear structure–adsorption relationships, highlighting how non-hexagonal motifs and curvature effects govern CO_2 affinity and retention under thermal agitation.

2. Computational Details

Reactive molecular dynamics simulations were carried out in LAMMPS [3] using the ReaxFF force field [4] to model the interactions between CO_2 molecules and carbon nanotubes constructed from distinct two-dimensional carbon allotropes, including Tolanene-NT and Pha-graphene-NT, alongside the reference CNT. For each system, the simulation cell was treated with periodic boundary conditions, and the temperature was controlled within the canonical (NVT) ensemble. Independent trajectories were generated at 100, 300, and 500 K to probe the thermal stability of adsorption and to distinguish between transient collisions and persistent binding events. CO_2 adsorption was quantified from the time evolution of the number of molecules retained in the vicinity of the nanotube surface, producing adsorption–time curves that enable direct comparison across nanotube topologies and temperatures.

5. Conclusions

The results indicate that CO_2 interacts weakly to moderately with the carbon nanotubes investigated, as evidenced by the progressive reduction in adsorption stability with increasing temperature. Among the studied systems, the Pha-graphene nanotube exhibits the strongest and most persistent CO_2 adsorption, showing enhanced thermal robustness relative to the other nanotubes. In contrast, the Tolanene nanotube displays comparatively weak CO_2 affinity, with limited and less stable adsorption across the simulated conditions.

6. References

[1] X. Chen, et. al., Carbon, vol. 170, pp. 477–486, 2020.

[2] Z. Wang, X.-F. Zhou, et. al., Nano Lett., vol. 15, no. 9, pp. 6182–6186, 2015.

[3] A. P. Thompson et al., Comput. Phys. Commun., vol. 271, p. 108171, 2022.

[4] A. C. T. van Duin, et. al., J. Phys. Chem. A, vol. 105, no. 41, pp. 9396–9409, 2001.

3. Results

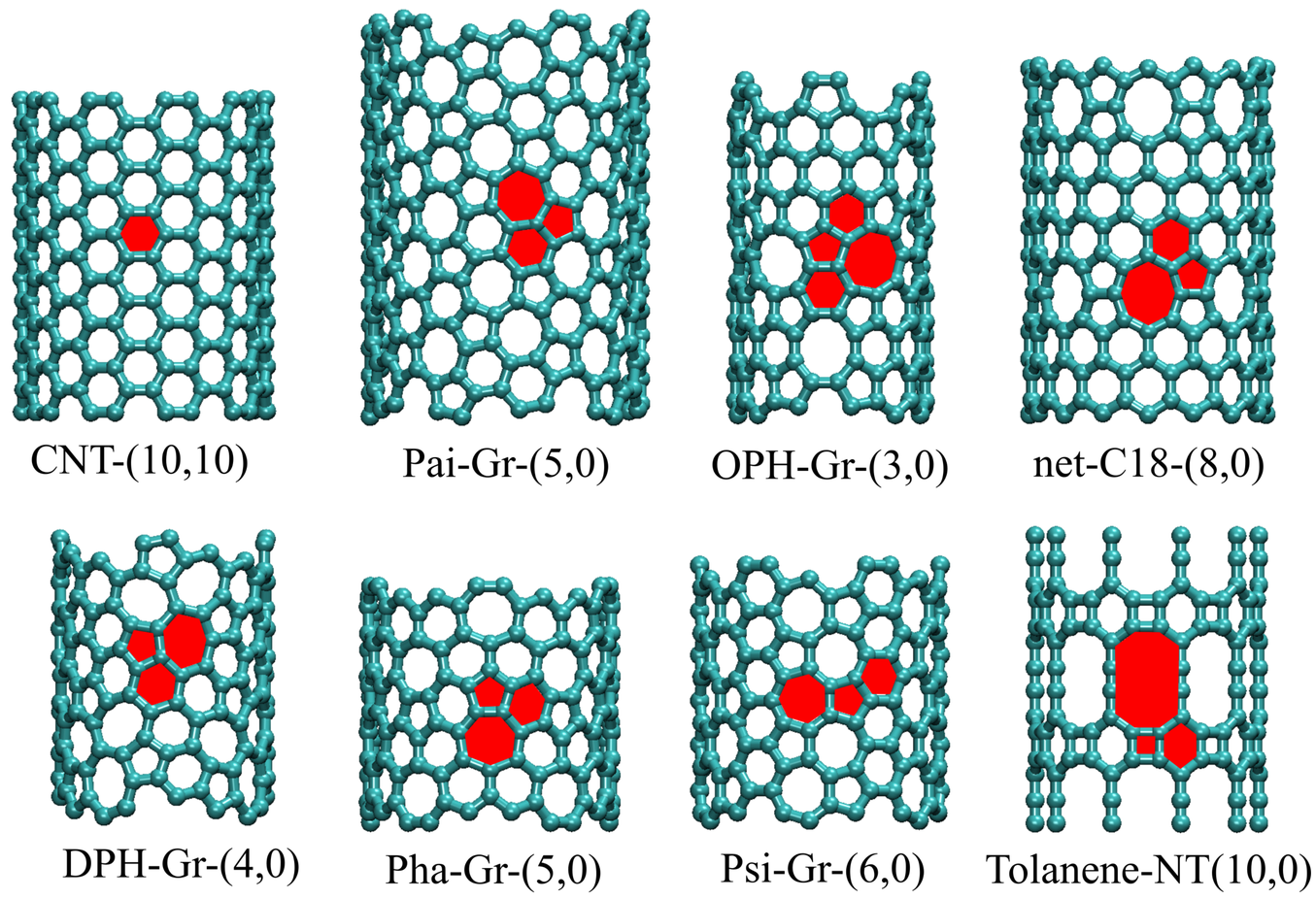

Figure 1. Representative atomic models of the nanotubes considered in this work, including the reference CNT(10,10) and nanotubes derived from non-hexagonal carbon allotropes (labels indicate the corresponding structures and chiral indices).

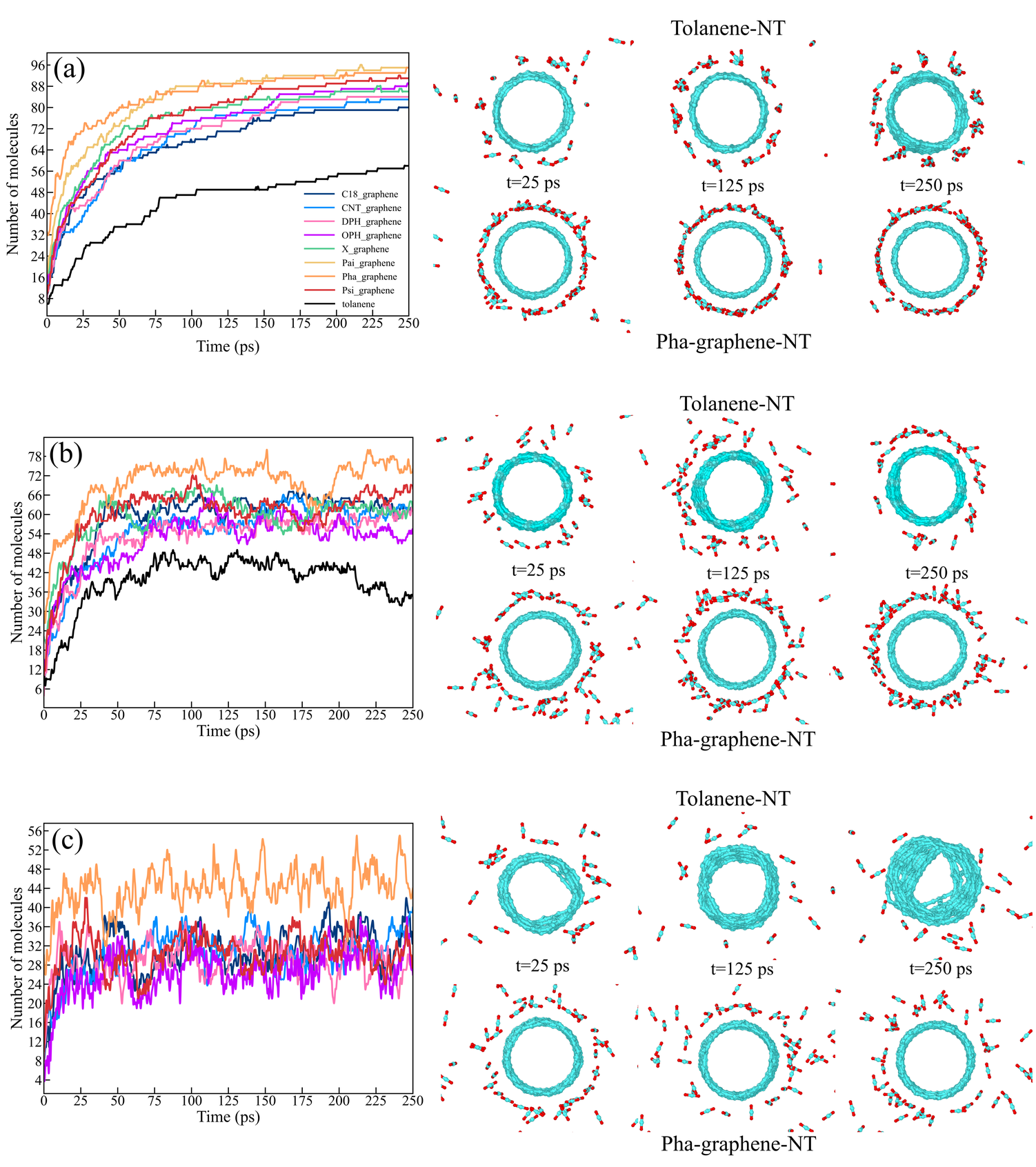

Figure 2. CO_2 adsorption as a function of time for the different nanotubes at (a) 100 K, (b) 300 K, and (c) 500 K. Selected snapshots for the Tolanene-NT and Pha-graphene-NT are shown at t = 25, 125, and 250 ps to illustrate the evolution of the adsorbed CO_2 configurations.