ATOMISTIC MOLECULAR DYNAMICS SIMULATIONS OF POLYMER NANOCOMPOSITES

A. J. Power[1,2,*], V. Harmandaris[1,2,3]

[1]Department of Mathematics and Applied Mathematics, University of Crete, GR-71409, Heraklion, Crete, Greece

[2]Institute of Applied and Computational Mathematics (IACM), Foundation for Research and Technology Hellas (FORTH), GR-71110 Heraklion, Crete, Greece

[3]Computation-based Science and Technology Research Center, The Cyprus Institute, Nicosia 2121, Cyprus

*ajpower@math.uoc.gr

ABSTRACT

Hybrid polymer/nanoparticle systems are a relatively new class of materials that has attracted growing scientific and technological interest [1-5]. In this work, the properties of polymer chains (PE and PEO) around of inorganic nanoparticles (pure Gold, grafted Gold and Silica) are investigated using classical atomistic molecular dynamics simulations. The structural, conformational, and dynamical properties of the chains were analyzed and compared to the behavior of the bulk polymer system. In more detail, we report data concerning polymer density profiles, bond order parameter, segmental and terminal dynamics. All properties are examined as a function of distance from the nanoparticles. A typical snapshot of the model systems is shown in (Fig. 1).

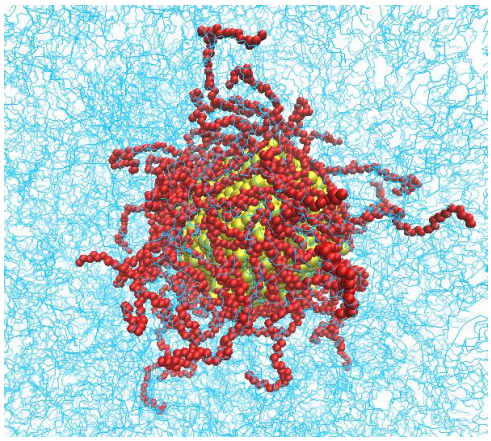
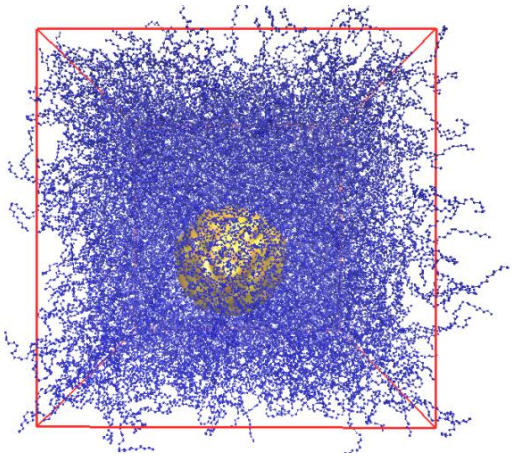
(a)  (b) 

Figure 1: **(a)** Hybrid PE/Grafted Gold Nanoparticle System; **(b)** Hybrid PEO/Silica Nanoparticle System.

KEYWORDS: nanoparticle, polymer, simulation, polyethylene, nanocomposite

REFERENCES

[1] Power, A.J., Remediakis, I.N., and Harmandaris, V. (2021). *Polymers,* 13(4): 541.
[2] Rissanou, A.N., Power, A.J., and Harmandaris, V. (2015). *Polymers*, 7: 390-417.
[3] Barmparis, G.D., and Remediakis, I.N. (2012). *Phys. Rev. B*, 86: 085457.
[4] Rissanou, A.N., Papananou, H., Petrakis, V.S., Doxastakis, M., Andrikopoulos, K.S., Voyiatzis, G., Chrissopoulou, K., Harmandaris, V., Anastasiadis, S.H. (2017). *Macromolecules,* 50 (16): 6273-6284.