# Molecular Dynamics Simulations of Surfactants Adsorption on Carbon Nanotubes Surfaces

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Abstract

During the last years, carbon nanotubes (CNTs) have been increasingly used in the fields of pharmacy and biomedicine [1, 2]. However, since it is an emerging technology, there is very limited information about their toxicity, complications or adverse reactions in the body. The other drawback to these structures is that they are very hydrophobic so that they cannot easily be handled in most solvents of biological interest. Different surfactants have been used to improve their dispersion in aqueous media [3]. In the present work, we investigated the adsorption behavior of two surfactants, sodium dodecyl sulfate (SDS) and sodium dodecyl benzene sulfonate (SDBS), at different concentrations on CNT surfaces by molecular dynamics (MD) simulations [4]. The results are presented in terms of distance between surfactant molecules and CNT surfaces, radial distribution functions and interaction energies. In all the models simulated here, a strong adsorption of both surfactants on CNT surfaces is seen as it is demonstrated by decreasing distances during simulation time and favorable energetic processes.

## References

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[2] A. Cerpa, M. Köber, D. Calle, V. Negri, JM Gavira, A. Hernanz, F. Briones, S. Cerdán, P. Ballesteros. Med. Chem. Com., 473 (2013) 270
[3] I. Lado Touriño, A. Cerpa Naranjo, V. Negri, S. Cerdán, P. Ballesteros, J. Mol. Graphics Modell., 62 (2015) 69
[4] [3] Materials Studio, (2016). Retrieved from http://accelrys.com/

## Figures

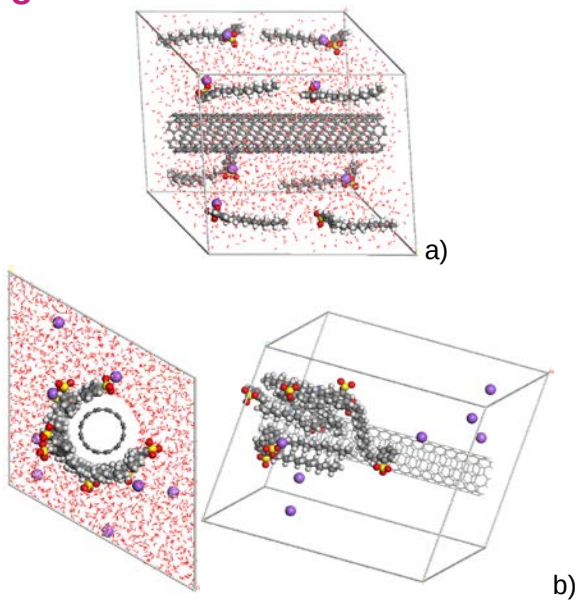


**Figure 1.** Initial (a) and final positions (b) of eight SDBS molecules interacting with a CNT obtained from molecular dynamics calculations. In part b) of this figure, two different views of the model are shown.

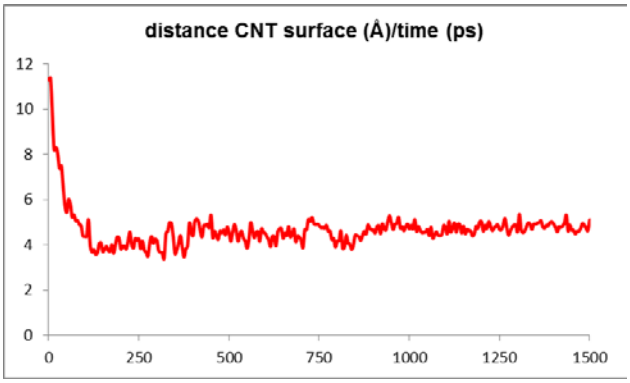


**Figure 2.** Evolution of the distance between the center of mass of SDBS molecules and the CNT surface with simulation time.