Diffusion of water molecules in CNT's functionalized with aminopyrene molecules

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Abstract
Magnetic Resonance Imaging (MRI) is currently one the most useful methods in clinical diagnosis. Its effectiveness may be improved by the design of new MR sequences highlighting the physiopathological properties of tissues and through the development of new Contrast Agents (CAs) increasing the quality, resolution and specificity of the MR images.[1] Diffusion tensor Imaging (DTI) is a recent methodology that allows the visualization of the white matter tracts underlying cerebral morphology and architecture. This methodology allows to study white matter diseases and has proven useful in the diagnosis of many neurological disorders, including demielinating diseases and ischemic and oncological processes. However, at present, there are not appropriate contrast agents to improve specificity and resolution of the DTI approach. We have previously shown that paramagnetic carbon nanotubes are able to perturb the diffusion of surrounding water molecules in an anisotropic manner, with larger effects in the longitudinal than in the transversal directions, constituting at present the first contrast agent for DTI.[2] However, the approach has remained limited by the reduced solubility of the nanotubes and the lack of sufficiently robust models to describe water diffusion in these systems. In this work we report recent progress in increasing solubility and paramagnetic character of CNTs obtained using pyrene adducts stabilized by−π stacking and Gd(III) derivatives of MWNTs. We focus then in the diffusional behavior of water molecules in the presence of the aminopyrene CNT adduct, to characterize the influence of various parameters such as length, diameter and concentration of carbon nanotubes and aminopyrene molecules. Our modeling study shows that the presence of CNT's modifies the diffusional behavior of water relative to bulk behavior and that diffusion of water molecules inside CNT's is slower than in the bulk solvent. Results on the distribution of water molecules in the interior of CNT's are also reported.

References

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(2) Negri, V., Cerpa, A.; López-Larrubia, P.; Nieto-Charques, L.; Cerdán, S.; Ballesteros, P., Angewandte Chemie Int. Ed. (2010) 49: 1813-1815.

Figures

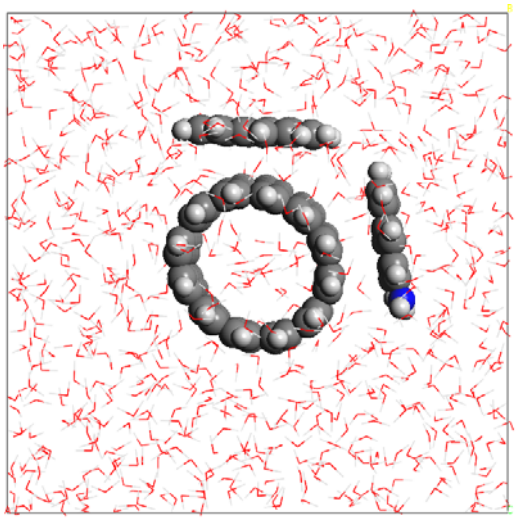

Figure 1. Model system used for the simulation of a CNT and two aminopyrene molecules in water.

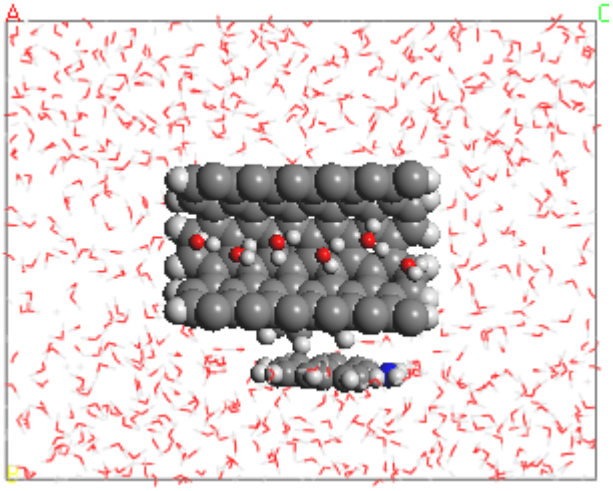

Figure 2. A snapshot from the simulation showing the structure of the hydrogen-bonded water chain inside the nanotube