Molecular dynamics simulation of the interaction between pure and functionalized carbon nanotubes and cement surfaces

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The theoretical study of the properties and structure of cement can be carried out by means of various molecular simulation techniques, among which the molecular dynamics method stand out, since it allows addressing the study of systems that, due to their chemical complexity, must be represented by a large number of atoms

In this work, we present the results of molecular dynamics simulation of the interaction between pure or functionalized single-walled carbon nanotubes (SWCNTs) or multiwalled carbon nanotubes (MWCNTs) and a representative cement surface (figure 1). The goal is to study the influence of the functionalization type of the CNTs on the interaction between the cement and CNTs, in order to reinforce this interaction, achieve a good CNTs dispersion and improve the mechanical properties of the cement, as well as analyze the differences obtained between SWCNTs and MWCNT.

Figures

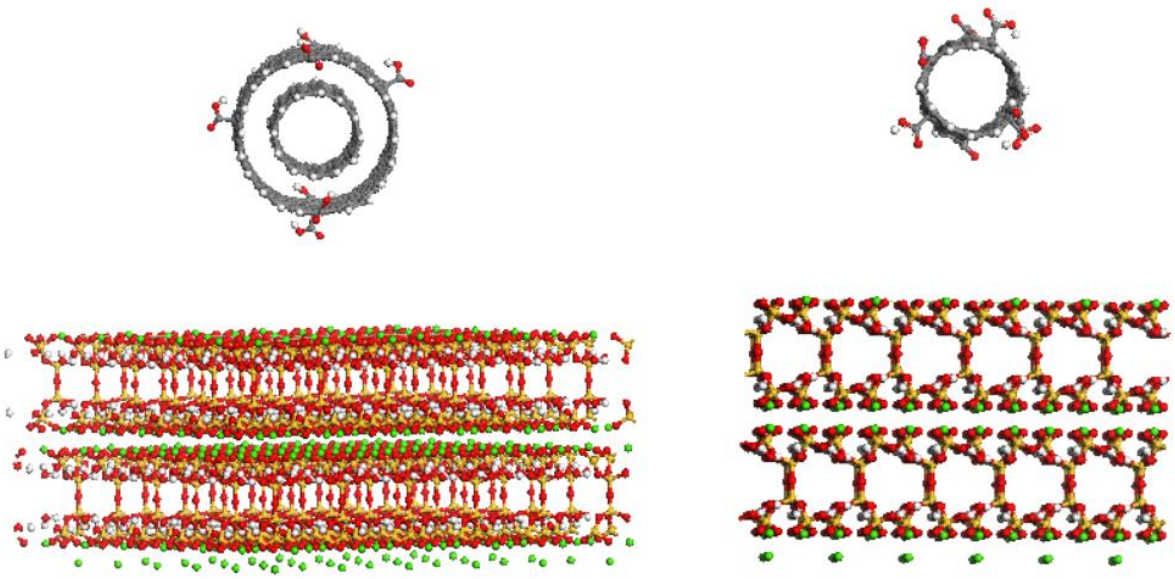

Figure 1. Two examples of functionalized carbon nanotubes interacting with the cement surface