A DFT STUDY OF THE INTERACTION OF SULFURIC ACID WITH BILAYER GRAPHENE

Isabel G. Ayala[1] and Nicolas A. Cordero[1,2]
[1] *Physics Department, University of Burgos, C/ Villadiego s/n, E-09001 Burgos, Spain*
[2]*Department of Materials Science and Engineering, University of Pennsylvania,*
3231 Walnut St, Philadelphia PA 19104, USA

ncordero@ubu.es

One of the main problems for the industrial application of single-walled carbon nanotubes (SWCNTs) is their insolubility in either water or organic solvents. The available methods for the synthesis of carbon nanotubes produce bundles of SWCNTs. It is necessary to disentangle these bundles in order to separate the tubes. There are many surfactant molecules suitable for this task, but among the best are sodium dodecyl sulfate (SDS), sodium dodecylbenzene sulfonate (NaDDBS), and sodium polystyrene sulfonate (NaPSS), all of which have in common a sulfonate head group. In fact, sulfuric acid itself is a good nanotube disperser, the proposed reason being the protonation of SWCNTs by this acid. We had previously studied the interaction of H_2SO_4 with a single graphene sheet (that can be seen as a very large radius SWCNT) and found this to be true [1], but in order to understand the surfactant effect it is necessary to analyze the way these molecules behave when in between two carbon nanostructures. We have used density functional theory (DFT) within the local density approximation (LDA) to calculate the interaction between sulfuric acid and bilayer graphene (i.e. H_2SO_4 molecules between two graphene sheets), calculating equilibrium geometries, binding energies, charge transfers and densities of states.

We have studied four different concentrations of H_2SO_4 ranging from nearly isolated acid molecules (Fig. 1) to two layers of H_2SO_4 (Fig. 2) between the two graphene sheets, namely one sulfuric acid molecule per 64, 36, 16 and 8 carbon atoms, respectively. Hexagonal and orthorhombic cells were chosen to take advantage of both graphene and sulfuric acid crystal symmetries.

References:

[1] N.A. Cordero and J.A. Alonso, Nanotechnology, **18** (2007) 485705.
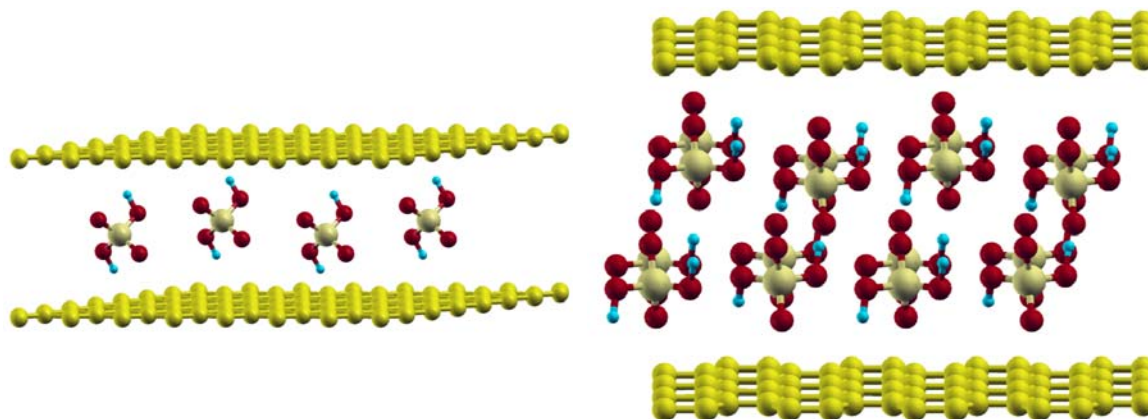
Figures:

Figure 1   Figure 2