A DFT study of the interaction of sodium bisulfate with monolayer graphene

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Large scale production of isolated carbon nanostructures (including graphene sheets) is important for nanotechnology progress. There are basically three approaches to separate carbon nanostructures: chemical functionalization, sonication, and the use of surfactants. Functionalization often changes de properties of the nanostructures and sonication breaks them. So the use of surfactants seems to be the best way to obtain isolated carbon nanostructures in large quantities. Among the best surfactant molecules for dispersing carbon nanostructures are sodium dodecyl sulfate (SDS), sodium dodecylbenzene sulfonate (NaDDBS) and sodium polystyrene sulfonate (NaPSS). All of them have in common a sulfonate head group with a Na atom. Sulfuric acid is itself a good surfactant, but the presence of a Na atom in the sulfuric group seems to enhance the surfactant effect. Our aim is to clarify the role this atom plays for dispersing carbon nanostructures.

We have previously studied the interaction of sulfuric acid with a graphene sheet [1], sulfuric acid, sodium bisulfate and sodium butyl sulfate with a carbon nanotube [2], as well as the behavior of sulfuric acid when in between two graphene sheets [3]. We present now computer simulations of the interaction between $NaHSO_4$ and monolayer graphene. We have used the Density Functional Theory (DFT) in the Local Density Approximation (LDA) as implemented in DACAPO [4]. We have calculated equilibrium geometries, binding energies, charge transfers and densities of states for different concentrations and orientations of both (cis and trans) $NaHSO_4$ isomers. Our results show that there is always protonation of the graphene sheet an that the charge transfer varies with bisulfate concentration and orientation.

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References

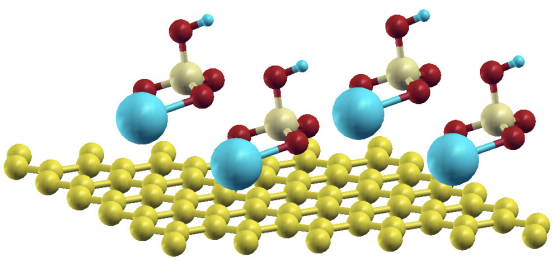
[1] N.A. Cordero and J.A. Alonso, Nanotechnology, **18**, (2007) 485705.

[2] N.A. Cordero and J.A. Alonso, Journal of Physical Chemistry C, **41**, (2010) 17249.

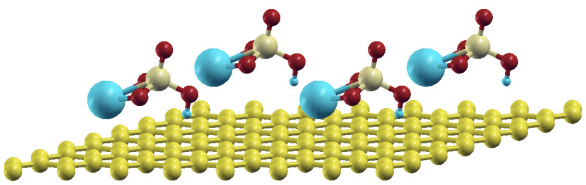
[3] I.G. Ayala, N.A. Cordero and J.A. Alonso, submitted to Physical Review B (2010).

[4] https://wiki.fysik.dtu.dk/dacapo/Dacapo

Figures



Medium concentration trans-$NaHSO_4$ over a graphene sheet



Low concentration cis-$NaHSO_4$ over a graphene sheet