Massimiliano Bartolomei
M. R. Cuevas-Flores, M. A. García-Revilla, C. Coletti
Instituto de Física Fundamental, CSIC, C/ Serrano 123, Madrid, Spain

maxbart@iff.csic.es

Interaction and reactivity of cisplatin physisorbed on graphene oxide prototypes

The physical adsorption of cisplatin (CP)[1] on graphene oxide (GO) and reduced graphene oxide (rGO) is investigated at the DFT level of theory by exploiting suitable molecular prototypes[2] representing the most probable adsorbing regions of GO and rGO platelets. The obtained results show that CP is preferentially adsorbed in correspondance of the epoxy and hydroxy groups (see Figure 1) and an energy decomposition analysis of the related binding energy reveals that the most attractive contribution comes from the electrostatic attraction between the $-NH_3$ ends of CP and the oxygen groups on the (r)GO basal plane. Moreover, it is found that the reactivity of the physically adsorbed CP is practically unaltered being the free energy variation related to the first hydration reaction almost matching that of its free (unadsorbed drug) counterpart[3]. The reported results suggest that overall the CP physical adsorption on GO and rGO carriers is feasible being an exergonic process in an aqueous medium. The CP adsorption could facilitate its solubility and transport in water solutions, exploiting the high hydrophilicity of the peripheral carboxylic acid groups located on the edge of the GO and rGO platelets.

References

[1] T. C. Johnstone, K. Suntharalingam, S. J. Lippard, *Chem. Rev.* 116 (2016) 3436
[2] M. R. Cuevas-Flores, M. A. Garcia-Revilla, and M. Bartolomei, *J. Comput. Chem.* 39 (2018) 71
[3] V. Graziani, C. Coletti, A. Marrone, N. Re, *J. Phys. Chem. A* 120 (2016) 5175

Figures

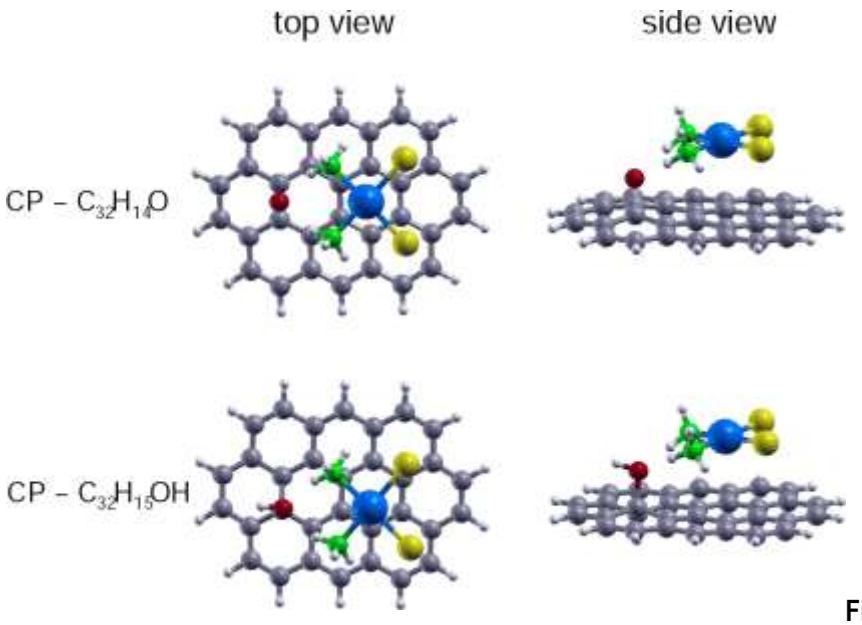

Figure 1: Top and side views of optimal molecular structures for CP physically adsorbed on (r)GO platelet prototypes.