Modelling the interaction between graphene surfaces and metallic nanoclusters

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Abstract

The overuse of antibiotics has led to the flourishment of antibiotic-resistant bacteria [1] and consequently to the need to develop new, more efficient pharmacological compounds. Several advanced materials are being studied, among which are metallic nanoparticles and certain graphene oxides (GO) modified with polyethylene glycol (PEG) [2-4]. In this work, molecular dynamics (MD) simulations of the adsorption of small Ag and Cu clusters on pristine graphene and PEGylated graphene oxide (GO_PEG) surfaces were carried out. The results are presented as a function of nanoparticles concentration, adsorption energies, mean equilibrium distances between nanoparticles and graphene surfaces (figure 1), radial distribution functions and diffusion coefficients of the metallic nanoclusters. These preliminary results show that PEGylation of the surface is critical to strengthen the interaction between the surfaces and the metallic clusters, which, in turn, is a key factor for improving the efficacy of these compounds.

References

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Figures

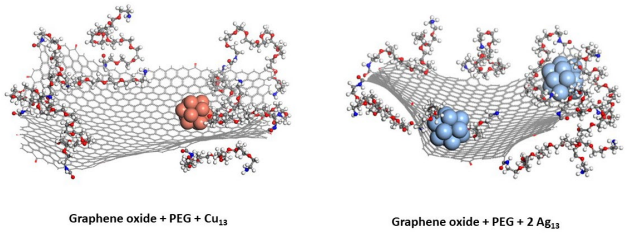

Figure 1: Final position of one Cu_{13} cluster and two Ag_{13} clusters on a PEGylated graphene oxide surface after 3 ns of simulation time.