NOVEL MORSE POTENTIAL TO STUDY THE Cu/C/H INTERACTIONS IN COPPER CAPPED BY GRAPHENE NANOPARTICLES TO PREVENT OXIDATION AND CORROSION

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ABSTRACT

During the last years, copper nanoparticles (Cu NPs) have attracted wide attention due to their many exploitable properties. One of the most outstanding is their strong biological activity, whichhase conferred multifaceted applications in biomedical and industrial fields including diagnostic, genetic engineering, pharmacology, agriculture and others.

Different investigations have demonstrated that when the size of the Cu NPs decreases, their biological activity is enhanced. However, this reduction in size also implies a higher superficial activity that favors phenomena such as oxidation and aggregation, changing or leading them to lose their properties. For these reasons, proper ways to prevent these phenomena and to manage the events occurring on their surface have been investigated.

Recently, copper nanoparticles capped by graphene (Cu@G NPs) have also attracted interest because graphene can serve as a shield to protect the Cu NPs from oxidation and corrosion and to improve their properties. Furthermore, graphene is an ideal candidate for coating Cu NPs due to its many advantages for biological applications, highlighting their remarkable biocidal activity with good biocompatibility and their sensitivity to the biochemical environment that allows the biofunctionalization by chemical species binding on their surface.

To date, many efforts have been made to understand the stability of small-size Cu NPs and Cu@G NPs. In addition to experimental techniques, high-performance computing assisted materials design has proved to be a powerful tool to gather physical insight from

different scales phenomena. It represents a powerful way to predict the feasibility and the properties of a system that can not be accessed in other ways, saving time, effort, and costs to the manufacturer.

In this work, we reported a novel Morse potential to study the stability of graphene flakes adsorbed on Cu NPs as a potential stabilizing agent against oxidation and corrosion. The fitting for Cu, C and H atoms was based on Density Functional Theory (DFT) calculations performed through Quantum Espresso/PWSCF, meanwhile the PBE generalized gradient approximation functional for the exchange-correlation term was adopted using the high-throughput GBRV pseudopotentials.

Morse potential parameters for atomic pairs involved in the flake-NP interaction were fitted taking DFT single point energies as a reference. Starting from a 1.5 nm Cu NP, only the first three layers of a (100) face and a (111) face were considered. On top of each face we added a planar and a pre-relaxed graphene flake large enough to cover them completely. Several single point energies were calculated, corresponding to different heights and lateral displacement of the flakes with respect to the surfaces.

Single point energies were also calculated using the resulting Morse potentials, with a very good agreement with the previously calculated DFT values. Additionally, molecular dynamics simulations were performed to evaluate the stability of the Cu@G NPs of different sizes. The obtained results were as was expected for this advanced nanomaterial taking into account the reported isolated properties of Cu NPs and graphene and from experimental stability studies of graphene adsorbed on Cu.