Advancing Nanomaterial Functionalisation: Stability and Dispersion of Metal Nanoclusters on PEGylated Graphene Oxide

Patrick Irigo[1], Miriam Roldán-Matilla[2], María Luisa Rojas-Cervantes[3], Mariana P. Arce[4], Javier Pérez-Piñeiro[4], María Fuencisla Gilsanz[4], Isabel Lado-Touriño[5*], Arisbel Cerpa-Naranjo[5*], Ren Guogang[1*]

[1]Technology Research Institute, University of Hertfordshire, Hatfield, Herts, UK.
[2]Professional Formation Centre. European University of Madrid, Villaviciosa de Odón, Madrid, Spain.
[3]Department of Inorganic and Technical Chemistry, Universidad Nacional de Educación a Distancia (UNED), Urbanización Monterrozas, Las Rozas, Madrid, Spain.
[4]Department of Science, Architecture, Engineering and Design Faculty. European University, Villaviciosa de Odón, Madrid, Spain.
[5]Department of Engineering. Architecture, Engineering and Design Faculty. European University, Villaviciosa de Odón, Madrid, Spain.

pi13aad@herts.ac.uk
arisbel.cerpa@universidadeuropea.es

Graphene and graphene oxide (GO) are increasingly utilised in energy, materials, and healthcare sectors [1], [2]. Silver (Ag) and copper (Cu) nanomaterials, including their nanoclusters, are pivotal for advanced antimicrobial therapies and enhancing materials for energy and biomedical applications [3]. However, achieving uniform dispersion and stability in both hydrophobic and hydrophilic environments remains a challenge [4]. This study addresses these challenges by synthesising and characterising PEGylated GO_{30} (30% oxidised) functionalised with Ag and Cu nanoclusters through amide bond formation. As shown in Figure 1, PEGylated GO_{30} stabilises Cu and Ag nanoclusters by providing steric effects and limiting aggregation. Using molecular dynamics (MD) simulations, we identified optimal strategies for stable nanostructures, focusing on radial distribution function (RDF) and mean squared displacement (MSD) analyses. The oxidation and subsequent PEGylation of graphene significantly enhance the interaction energy of Ag nanoclusters by 239.47 kcal/mol and Cu nanoclusters by 259.98 kcal/mol. This functionalisation also substantially reduces nanocluster mobility, with MSD values of 20-30 $Å^2$ at 500 ps, compared to 150-175 $Å^2$ for non-functionalised clusters. RDF analysis reveals improved nanocluster dispersion on the PEGylated GO_{30} surface, supporting the formation of stable nanostructures. SEM and TEM analyses corroborate these findings, showing that PEGylation enhances nanoparticle dispersion and reduces aggregation on GO_{30} sheets, achieving a more consistent size distribution of 10-20 nm. UV-Vis spectroscopy indicates that PEGylated Ag nanoparticles exhibit a stable plasmonic response between 400-450 nm, which is crucial for their antimicrobial activity.

Overall, PEGylation significantly enhances the stability, dispersion, and antimicrobial functionality of metal nanoclusters on graphene-based materials, underscoring their potential for drug delivery, antimicrobial technologies, and sensing applications, while laying a strong foundation for future research in functional nanomaterials.

References

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Figure

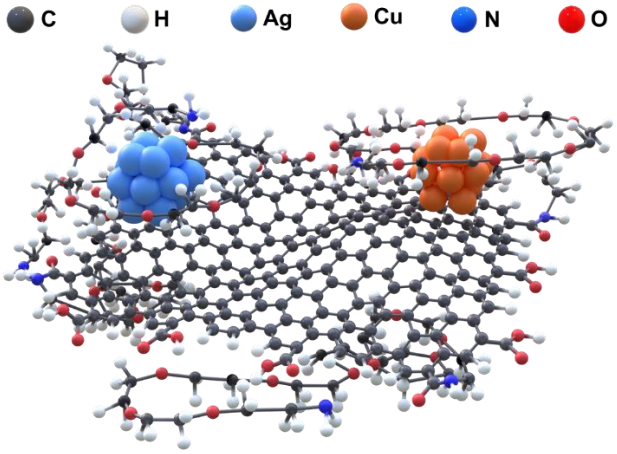

Figure 1. GO_{30} functionalised with PEG-NH_2 stabilises both Cu and Ag nanoclusters. The PEG chains provide steric stabilisation, preventing nanocluster movement along the GO_{30} sheets and limit aggregation by creating a physical barrier, reducing the likelihood of aggregation.