

Composite films of waterborne polyurethane and few-layer graphene formed in water by stabilization with a pyrene derivative

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Abstract

The search for graphene or few layer graphene production methods that are simple, allow mass production and yield good quality material continues to motivate intense investigation. The present work reports the study of the exfoliation of graphite in an aqueous solution of a soluble pyrene derivative (PY) that was synthesized to achieve maximum interaction with the graphene surface at a low concentration of 5×10^{-5} M (Figure 1). [1] Four graphite/graphite nanoplatelets with different morphologies and geographical origin were tested. The yield of bilayer and few layer graphene (FLG) obtained in suspension was quantified by UV-Vis and Raman spectroscopic analysis and the adsorption of PY on the graphene surface was studied by thermogravimetric analysis. Molecular modelling of the adsorption process allowed the calculation of the binding energy of the PY on graphene. The model demonstrates that the graphene surface can accommodate a maximum of 1 PY molecule per 34 graphene carbon atoms, as represented in Figure 2.

Composite films of waterborne polyurethane (WPU) and FLG were

produced by spray coating. The dispersion of the FLG was analysed by Raman mapping and electron microscopy. The films were tensile tested, showing an increase in Young's modulus and tensile strength of approximately 50 and 20 %, respectively, for films containing 0.5 wt% of FLG. At this composition, the water vapour permeability reduced by approximately 40% and the electrical resistivity dropped by three orders of magnitude.

References

- [1] C. Silva, S. Caridade, E. Cunha, M.P. Sousa, H. Rocha, J.F. Mano, M.C. Paiva, N.M. Alves, *Macromol. Mater. Eng.*, (2018) 1700316.

Figures

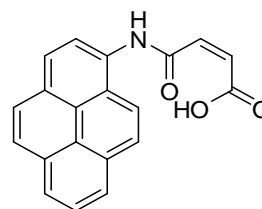


Figure 1: Chemical structure of the synthesised pyrene derivative

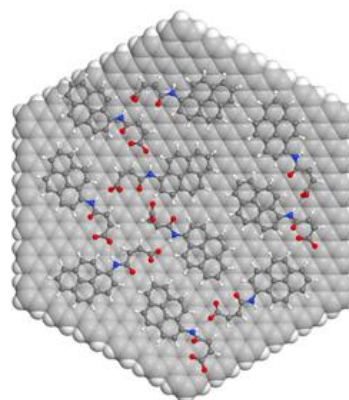


Figure 2: Model with 10 deprotonated PY molecules adsorbed on a graphene monolayer flake at the GFN-xTB level. The graphene flake is represented by an array of carbon spheres and the PY molecules are shown with the ball and stick representation.