Towards The Development of a QSAR Approach to High Concentration Graphene and Reduced graphene Oxide Dispersions Exfoliation

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The stable dispersion of graphene in polar solvents such as water requires the use of stabiliser molecules. Desirable properties of such dispersions include low excess stabiliser content, high graphene concentration and large flake size. Polyaromatic sulphonic acid salts have shown promise in meeting these criteria, adsorbing onto graphene through π-π interaction. In our study, we present a series of perylene, pyrene and triphenylene monofunctional amphiphilic molecules with different alkyl and alkynyl chain lengths between the ionic head and polyaromatic core have been synthesised and systematically tested on the *in-situ* reduction and stabilisation of graphene oxide. The effect of spacer and core both influence the final concentration of these materials, with perylene core groups showing the highest efficiency. Combination of this with an unsaturated alkynyl chain and sulphonic acid salt, produces quantitative yields of 100% monolayer aqueous reduced graphene oxide dispersions with no reduction in flake size. The application of this material for inkjet printing and elastomeric composites is also shown.