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Different molecular interactions of graphene sheet and quantum dot nanomaterials

Thanks to its extraordinary properties, graphene attracts much research and applications interest. The rich π-system and high surface area of graphene are attractive for non-covalent interactions, but their structural and electronic nature is complex and remains unclear, particularly in solvents including water. Hydrophobic and π-π stacking interactions are often reported as their driving force [1, 2], but the nature of interaction may be misunderstood from surface characterisation and computational modelling done in the absence of water. Where water has been included in fewer studies, very different behaviour is reported [3, 4]. Here, we investigated the molecular nature of interactions of graphene sheets and quantum dots in water using NMR spectroscopy, and develop a mechanistic model to explain the major differences in interactions revealed. Self-assembly of aromatic compounds is revealed by large upfield shifts of 1H NMR signals due to the orbital diamagnetism of aromatic ring currents. The large orbital diamagnetism of graphene aligns planar π-π assembly in the magnetic field and thereby depletes signals without shift, whereas remaining signals are un-shifted but broadened (Figure 1), indicating unaligned non-planar association with graphene and different interactions of chemically-diverse structures with graphene surfaces and edges. As the size and orbital diamagnetism of graphene decreased into quantum dots with greater disorder, planar and non-planar molecular interactions were markedly less.

References

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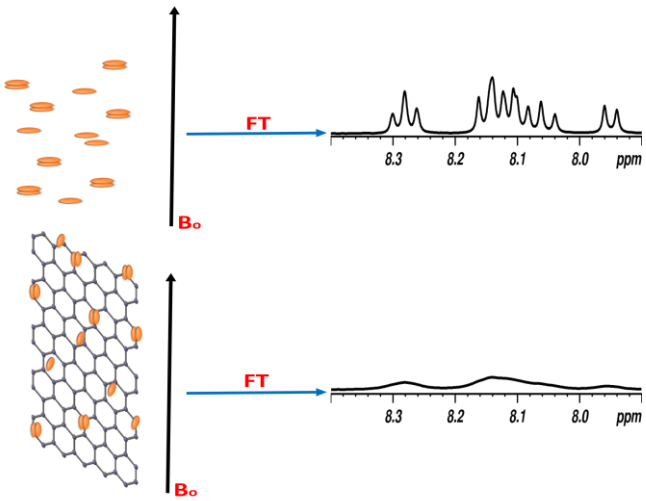

Figure 1: Effect of graphene on ^{1}H-NMR spectra. Chemical shifts of ^{1}H protons of aromatic compounds in the absence (top) and presence (bottom) of graphene.