## **Electronic Supplementary Information**

## Graphene quantum dots: effect of size, composition and curvature on their assembly

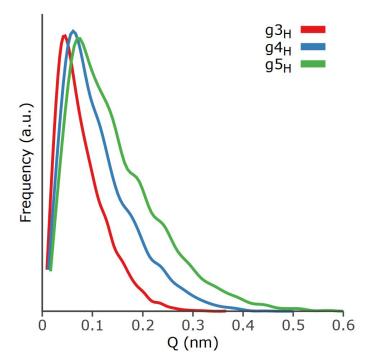
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**Figure X1** Measure of the deviation from a planar configuration for hydrogen terminated single GQDs of different sizes.

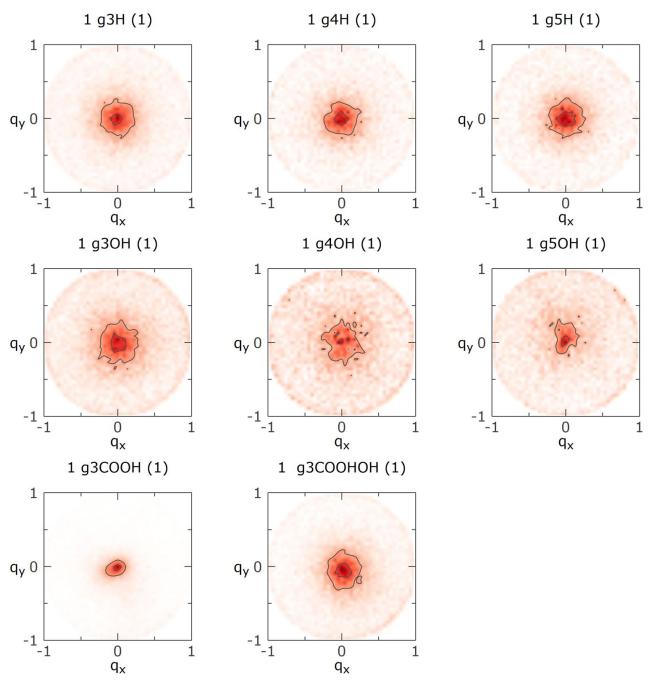
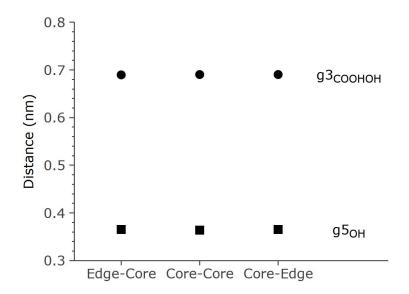
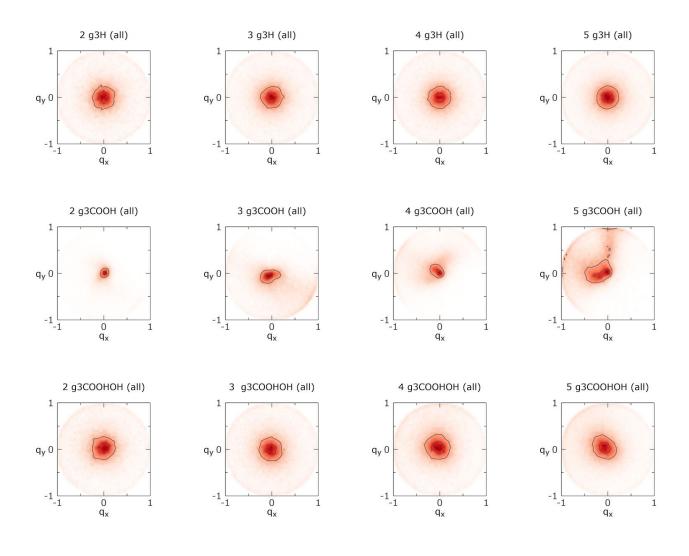


Figure X2 Distribution of conformations of single GQDs in water.



**Figure X3** Dependency of the interlayer distances on the relative position of the molecules inside a 4 GQDs stack. Both stacks are composed entirely by the same type of structures CS for the g5OH and WS for the g3COOH.OH. Errorbars are smaller than the symbols.



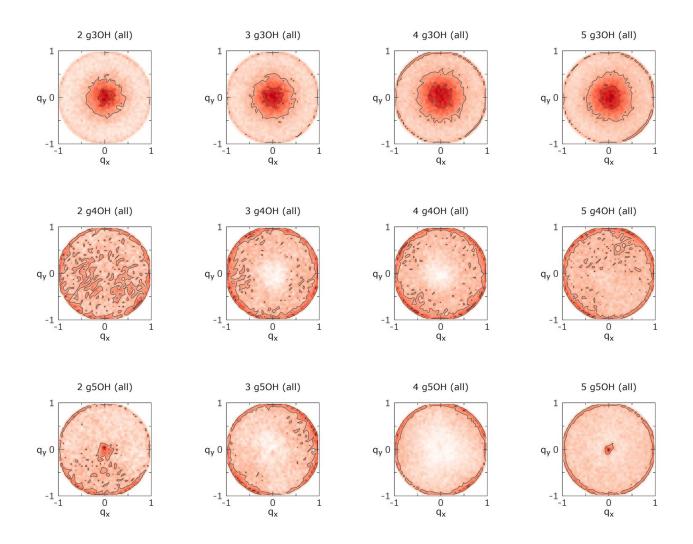


Figure X4 Distribution of conformations of aggregated GQDs in water. These are the average of all the configuration during the simulations of all the