Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Evidence of benzenoid domains in nanographenes

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ELECTRONIC SUPPLEMENTARY INFORMATION

ESI1. Optimized geometry of hexagonal-shaped A-GQDs, non-hexagonal A-GQDs and hexagonal-shaped Z-GQDs.

ESI2. Algorithm for generating the GQDs samples of Fig. 3.

ESI3. Comparison between calculations performed with the PBE and B3LYP exchange-correlation functional.

ESI1. Optimized geometry of hexagonal-shaped A-GQDs, non-hexagonal A-GQDs and hexagonal-shaped Z-GQDs.

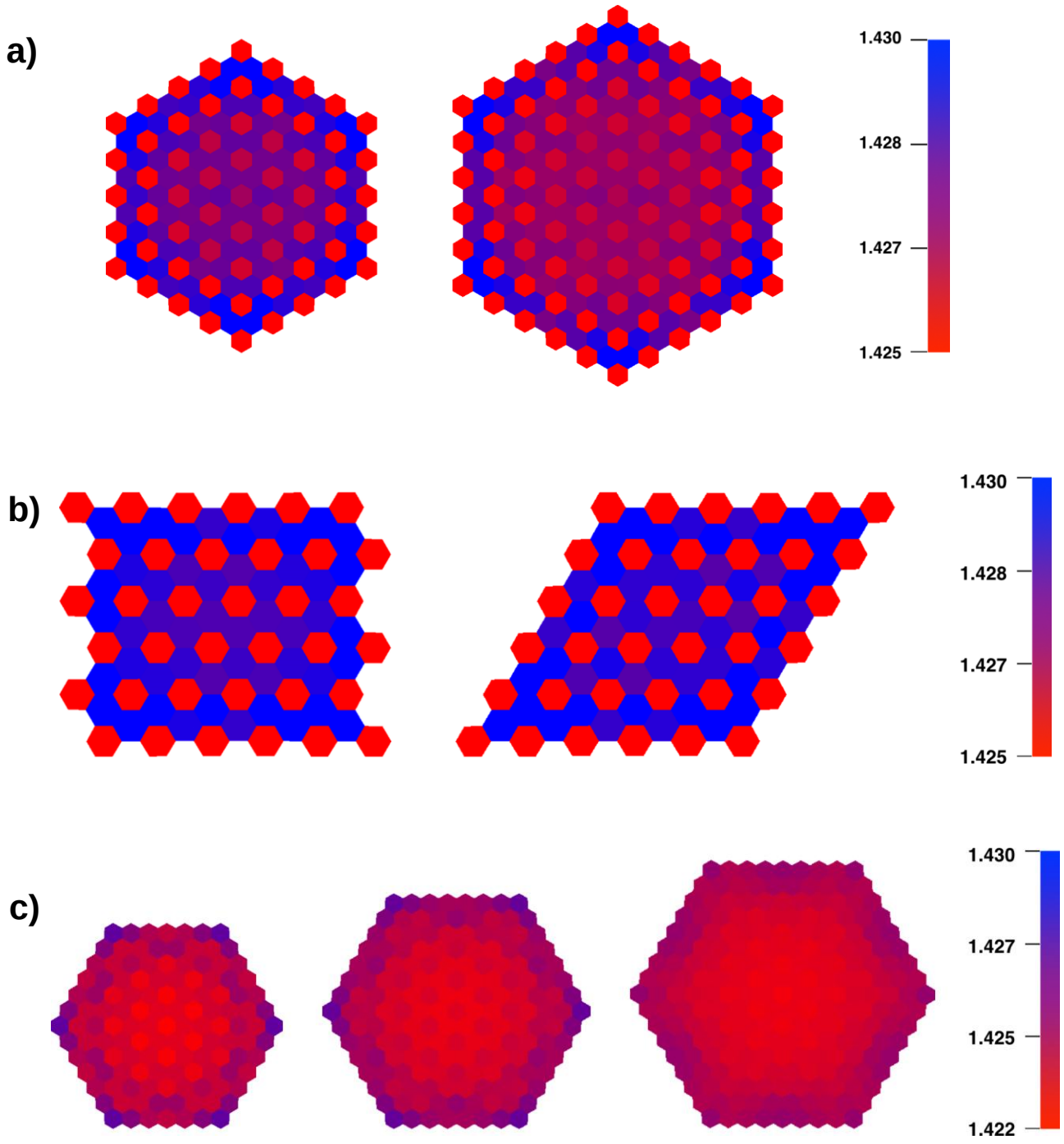

Figure ESI1. Optimized geometry of a) hexagonal-shaped A-GQDs; b) non-hexagonal-shaped A-GQDs and c) hexagonal-shaped Z-GQDs. Six-membered rings are color-coded according to their MBL; values in the scale bar are in Å.

ESI2. Algorithm for generating the GQD samples of Fig. 3

The samples in Fig. 3 are constructed by generating the convex hull of a set of points taken from a regular honeycomb lattice. These points are selected from the region defined by a set of lines, with random orientation and displacement with respect to the origin of the underlying hexagonal lattice, until a closed polygon is generated. This step is represented in Fig. ESI2a and the resulting closed polygon is shown in Fig. ESI2b. In this step, only lines with at least one intersection with other lines are considered. The morphology of the GQD is then defined by all the six-membered rings enclosed[1] within the polygon, as in Fig. ESI2c.

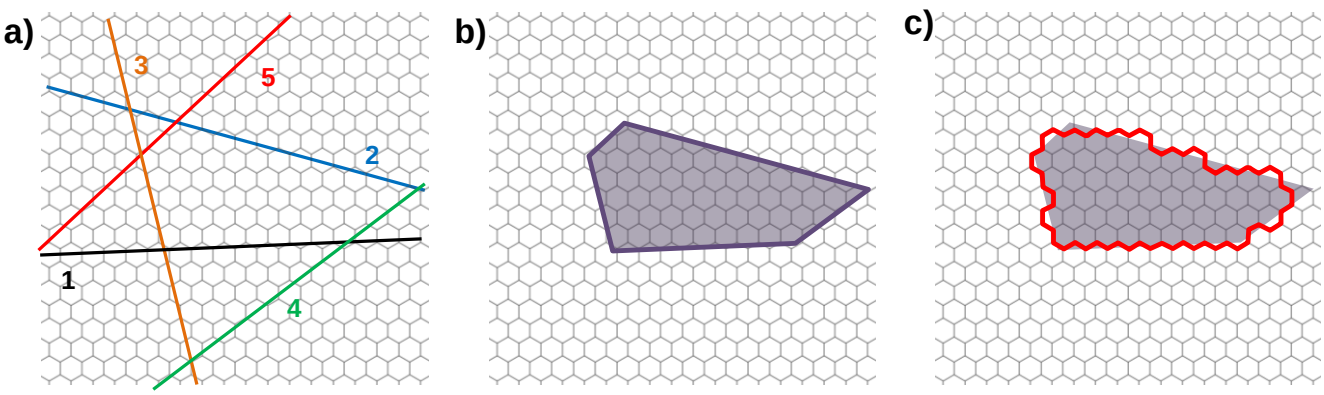

Figure ESI2. a) Generation of a set of lines with random orientation and displacement with respect to the underlying hexagonal lattice. Labels and colors represent successive generation of lines until a closed polygon is formed. b) The resulting closed polygon. c) Generation of the GQD morphology.

[1] A six-membered ring is considered as enclosed within the generated polygon if 50% or more of its area overlaps with the area of the polygon.

ESI3. Comparison between calculations performed with the PBE and B3LYP exchange-correlation functional

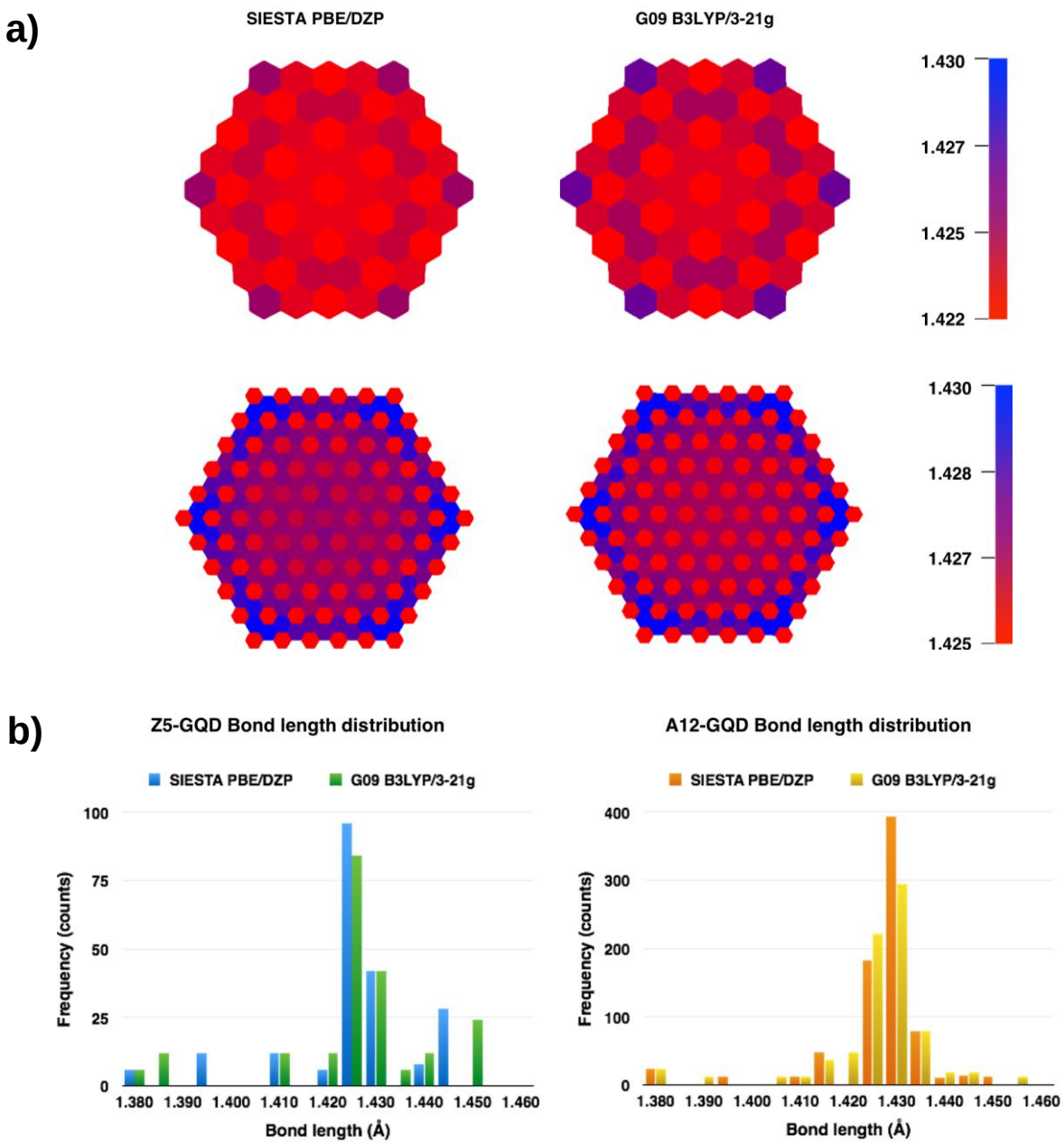

Figure S3. a) Optimized geometries of Z5-GQDs (top) and A12-GQDs (bottom) as computed with the Siesta program package, PBE exchange correlation functional and a double-ς plus polarization (DZP) basis set (left) and with the Gaussian09 (G09) program package, B3LYP exchange-correlation functional and 3-21g basis set (right). Six-membered rings are color-coded according to their MBL; values in the scale bar are in Å. b) Histogram of C-C distances in the Z5-GQD (left) and A12-GQD (right) computed at the two levels of theory.