Electronic and transport properties of chemically functionalized nanographenes

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Recent advancements in production techniques have allowed the synthesis and characterization of novel nanostructured materials based on graphene.[1] Particularly, recent research efforts have been targeted to the investigations of low-dimensional nanographenes, such as graphene quantum-dots (GQDs) and nanoribbons (GNRs). Here, the dimensional confinement at the nanoscale allows the tuning of the intrinsic electronic properties of graphene, which can potentially be exploited for the production of next-generation nanostructured electronic devices. Nevertheless, limitations in current experimental methodologies hinder both the controlled synthesis of nanographenes, with well-defined electronic properties, and large-scale production. To overcome these issues, the chemical modification of graphenes has been spotted as a viable route to produce materials with controlled and well-defined properties with potential use in applications. However, despite recent theoretical and experimental efforts,[2,3] a comprehensive understanding of the relationships between chemical structure and electronic properties in nanostructured graphenes is still missing. This concern is particularly critical in relation to the electron transport properties of chemically-modified graphenes, in view of their use in nanoelectronics.

In this work, we analyze, by means of density functional theory and non-equilibrium Green's function calculations, the electronic and transport properties of low-dimensional graphene nanostructures subjected to chemical functionalization. Our calculations concern models based on GQDs, GNRs and functionalized nanostructures thereof, targeting systems of interest in recent experiments, focused on oxidization and edge-functionalization of nanographenes.[4] In particular, we demonstrate how the remarkably versatile chemistry of sp^2 carbon and the use of traditional organic chemistry concepts[5,6] provide a reliable guide to rationalize the properties of chemically functionalized graphenes. The application of rigorous concepts in the definition of model systems and the use of high-performance computing platforms constitute crucial prerequisites for realistic simulations of low-dimensional carbon nanostructures aimed at the development of novel materials with potential application in nanoelectronics.

References

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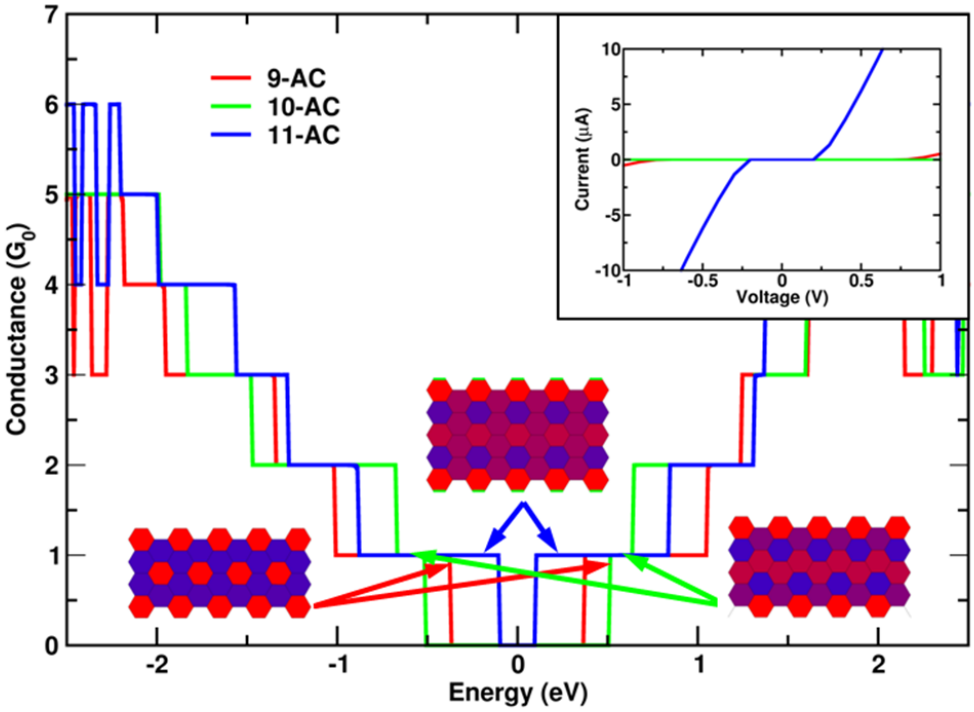
Figures



Transmission spectra and I(V) characteristics (inset) of armchair-edge 9-AC (red lines), 10-AC (green lines) and 11-AC (blue lines) GNRs. Optimized structures, color-coded according to their mean bond length (average of the six C-C bond lengths for each six-term ring), are also depicted above the corresponding transmission plateau.