Atomistic control of the properties of nanographenes and design of devices: insights from simulations

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The electronic properties of graphene can be fine-tuned through a careful control of the morphology at the nanoscale or by chemical functionalization, thus opening exciting perspectives for the development of novel devices for nanoelectronics. However, a comprehensive understanding of the key factors governing the relationships between morphology of nanographenes at the microscopic scale and potential functionalities is still in early stage of development.[1]

In this work, we explore the correlation between the atomistic structure and the properties of systems based on graphene by extending concepts borrowed from traditional organic chemistry corroborated by accurate theoretical calculations using density functional theory. Namely, we perform calculations on realistic models to rationalize the structural, electronic and transport properties of nanographenes and related systems.[2] The approach proposed allows to elucidate recent experimental observations on the effect of morphological details of graphene nanoflakes and nanoribbons on their properties beyond idealized models and provides viable synthetic routes for the design and synthesis of novel systems with tailored properties. Moreover, similar concepts are also applied to the design of nanostructured devices, based on functionalized nanographenes, able to perform basic operations through the application of external inputs.[3] In particular, we demonstrate the potential of our approach in the design of a reversible switch, based on functionalized graphene nanoribbons, exhibiting unprecedented ON/OFF ratios upon application of an external redox potential.

The study presented points out the need for a precise control of the atomistic structure of systems based on graphene and, at the same time, suggests efficient routes for the design and optimization of novel materials, with controlled morphology and properties, which can be used in technological applications.

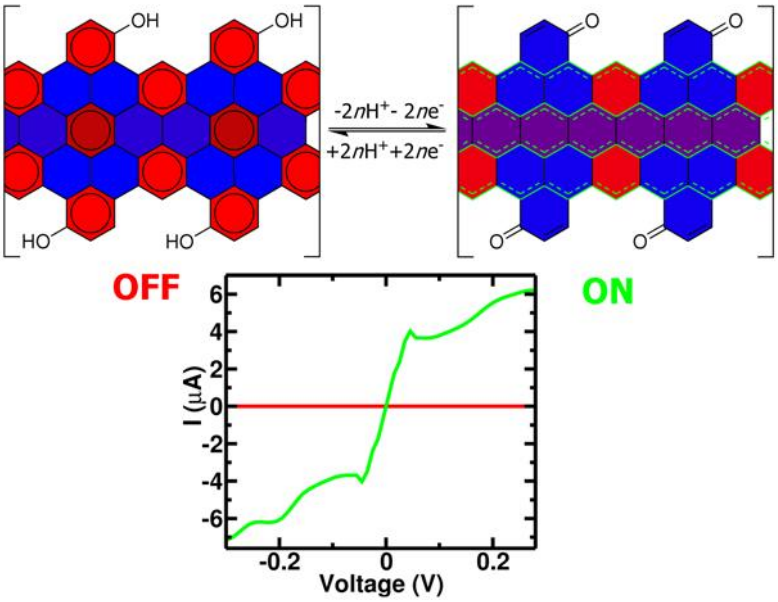
References

[1] M. Baldoni, A. Sgamellotti, F. Mercuri, Chem. Phys. Lett, **464** (2008) 202.

[2] F. Mercuri, M. Baldoni, A. Sgamellotti, Nanoscale, **4** (2012) 369.

[3] D. Selli, M. Baldoni, A. Sgamellotti, F. Mercuri, Nanoscale, **4** (2012) 1350.

Figures



Reduced (left) and oxidized (right) forms of a reversible switch based on a functionalized graphene nanoribbon and corresponding I(V) characteristics (bottom) showing the ON/OFF ratio.