Ab initio insights into the electronic properties of 1D and 2D porous carbon-based nanoarchitectures

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In recent years, a wide selection of atomically-precise carbon-based nanoarchitectures has been created using on-surface synthesis (OSS) techniques. [1,2] Remarkably, it is now possible to obtain carbon-based materials using allotropes other than graphene, such as biphenylene. [3] This emerges as a new degree of freedom to tune the electronic properties of such 1D and 2D materials. In this work, we employ Density Functional Theory (DFT) to explore how the electronic properties of 1D and 2D carbon-based nanoarchitectures are modified by the inclusion of graphene-like and biphenylene-like units. In particular, we focus on porous 12-atoms-wide armchair graphene nanorribons (12-PGNR), and on the 2D nanoporous networks that would emerge from their lateral fusion. The nature of this lateral fusion, either graphene-like or biphenylene-like, greatly affects the electronic properties of the resulting 2D system. Our results will be useful to interpret Scanning Tunneling Microscope (STM) and Atomic Force Microscope (AFM) experiments performed by our collaborators.

[1] César Moreno et al, Science, 360 (2018),6350.
[2] Wenhui Niu et al., Angew. Chem. Int. Ed., 62 (2023), e202305737.
[3] Qitang Fan et al., Science, 372 (2021), 6544.

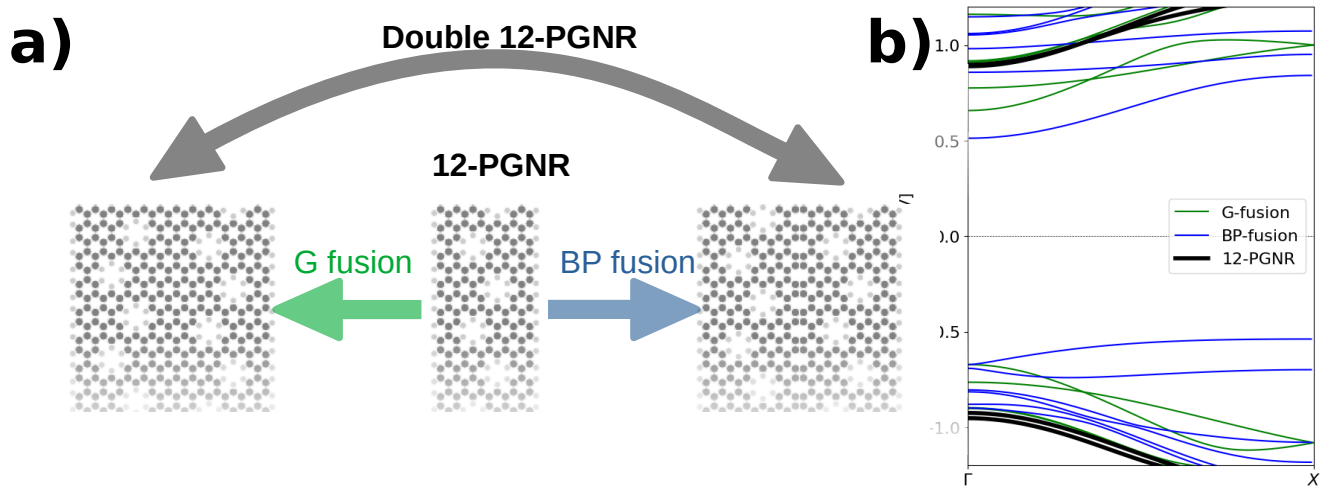

Figure 1. a) Atomic structures that arise from graphene-like (left) and biphenylene-like (right) lateral fusion of two 12-PGNRs (centre). **b)** Electronic band structures of the systems shown in a), where the different electronic behaviors can be clearly observed.