Magnetism in carbon nanoarchitectures: from 1D to 2D

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Recent progress in on-surface synthesis (OSS) has made it possible to obtain atomically-precise bottom-up nanoporous graphene (NPG) structures by laterally fusing 1D graphene nanoribbons (GNRs). [1] Besides, it has been demonstrated that GNRs can host localized spin states by chemical substitution with boron atoms. [2,3] Within this scenario, the lateral fusion of such magnetic GNRs emerges as a promising route to achieve 2D magnetic nanoarchitectures.

In this work, we employ Density Functional Theory (DFT) to explore how the electronic and magnetic properties of boron-doped graphene nanoarchitectures are modified with varying dimensionality from 1D to 2D. In particular, we focus on boron-doped armchair graphene nanoribbons that combine 5 and 11 C-atom wide segments, and on the 2D nanoporous networks that would emerge from their lateral fusion. The proposed structures combine a metallic character with the presence of S=1/2 spin states in its interior. Our results might be of great interest for the ongoing research of 2D graphene-based magnetic nanoarchitectures.

References

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[3] N. Friedrich *et al*. , ACS Nano **16**, 14819 (2022).

Figures

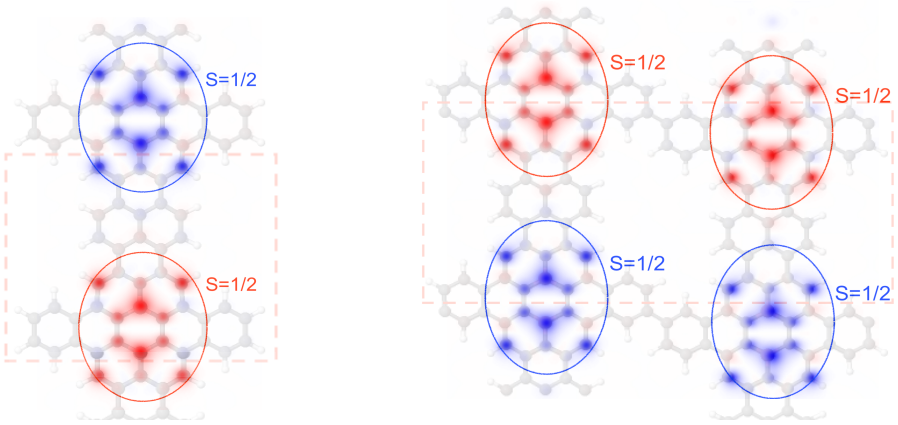

Figure 1: Spin-polarized density maps superimposed on the corresponding atomic structure of a model B-doped GNR (left) and the corresponding NPG (right), which hold S=1/2 spin states localized around the borylated regions. The red dashed rectangles show the unit cell of each structure.