Boron Substitution in Graphene Nanoribbons: Onedimensional Spin Chains with Tuneable Interactions

N Friedrich¹, P Brandimarte², J Li¹, S Saito³, S Yamaguchi⁴, I Pozo⁵, D Peña⁵, T Frederiksen^{2,6}, A García-Lekue^{2,6}, JI Pascual^{1,6} and **D Sánchez-Portal^{1,7}**

¹ CIC nanoGUNE BRTA, Donostia (Spain)
² DIPC, Donostia (Spain)
³ Kyoto University, Kyoto (Japan)
⁴ Nagoya University, Nagoya (Japan)
⁵ CiQUS, Univ. Santiago de Compostela (Spain)
⁶ Ikerbasque, Bilbao (Spain)
⁷ CFM CSIC-UPV/EHU, Donostia (Spain)

daniel.sanchez@ehu.es

Graphene nanoribbons (GNRs), lowdimensional platforms for carbon-based electronics, show the promising perspective to also incorporate spin polarization in their conjugated electron system. However, these magnetic moments are usually localized around ziazaa edges, difficult to fabricate and very reactive. This combined theoretical and experimental study demonstrates that magnetism can also be induced away from physical edges through atomically precise engineering of topological defects in its interior. A pair of substitutional boron atoms inserted in the carbon backbone of the 7armchairGNR breaks the conjugation of its topological bands and builds two spinpolarized boundary states around them. Therefore, a spin moment of 2 Bohr magnetons localizes around each pair of B atoms in the structure (see Figure 1).

First indications of the presence of magnetism were given by the appearance of characteristic Kondo peaks in electrical performed experiments transport at nanoGUNE. Transport was measured through boron-substituted GNRs suspended between the tip and the sample of a scanning tunnelina microscope (STM). These observations were rationalized in terms of the theory and first-principles simulations performed at CFM and DIPC, which predicted for each isolated boron pair a S=1 spin state as well as a strong dependence on

the spacing between pairs. The interaction between two of such topological defects was further explored, outlining a route to engineer topological spin chains, with the promising tunability of their magnetism by modifying their spacing [1].

Therefore, the present results demonstrate a route to embed spin chains in graphene nanoribbons, turning them into basic elements of spintronic devices. We are currently examining the effect of B substitution for other GNRs.

References

[1] N. Friedrich et al., Physical Review Letters 125 (2020) 146801

Figures



Figure 1: a) Structure of the 2B-7AGNR defect together with the computed spin density map. b) Constant height STM scan (V=2 mV) using a CO-functionalized tip of a 2B-7AGNR defect.