Enhancing and tuning the magnetic response in graphene nanoribbons by means of straintronics and adatoms

Pablo Moles Matías
Hernán Santos, Francisco Domínguez-Adame and Leonor Chico
Universidad Complutense de Madrid, Avenida Complutense s/n, 28040, Madrid, Spain
pmoles@ucm.es

The possibility that a non-magnetic material such as graphene could exhibit magnetism stemming from pz orbitals has attracted the attention of researchers for more than a decade. Graphene nanoribbons with zigzag edges are regarded as one of the most intriguing systems for investigation. Theoretically, unlike bulk graphene, they are anticipated to display intrinsic magnetism due to the spin polarization of their edge states, making them ideal for spintronics. However, the detection of this edge magnetism remains challenging, as structural defects at the edges of synthesized ribbons appear to dampen the magnetic response, a phenomenon highly sensitive to the atomic precision of the edges.
In this work we present the possibility of increasing the magnetic response of zigzag graphene nanoribbons by applying strain in the longitudinal direction of the ribbon. This could facilitate the experimental detection of magnetism. We perform DFT calculations, which are compared with a tight-binding Hubbard Model in mean field approximation, that allows great versatility and scalability of the calculations. Both models fit together with remarkable precision. As a result of the modification of the bands, increases in magnetization close to 90% are obtained at strain values of 15%.
We also study the possibilities of modifying magnetism through the selective deposition of Hydrogen adatoms, combined with strain. These are already experimentally handled with atomic precision in graphene and can also help to better understand the magnetic dependence on defects.

References

[1] Huang, B. et al. (2008). Physical Review B, 77(15), 153411
[2] Brede, J. et al. (2023). Nature Communications, 14(1), 6677
[3] González-Herrero, H. et al. (2016). Science 352.6284, 437-441

Figures

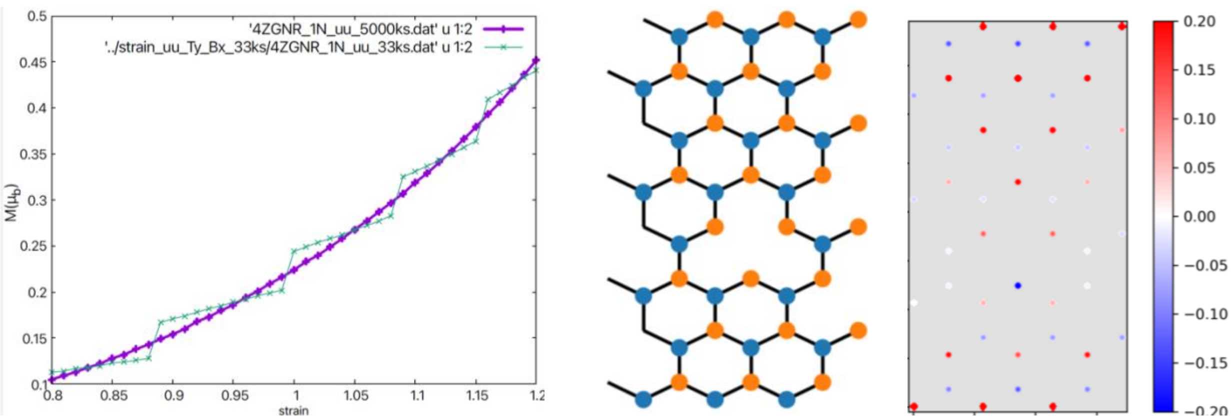

Figure 1: Left: Magnetic moment of an edge atom as a function of strain. Center: system with a vacancy and a 15% of applied strain. Right: Resultant magnetization from the previous system