Predicting magnetic edge behaviour in graphene using neural networks

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A large number of proposed spintronic devices are predicated on the formation of local magnetic moments near the edges of graphene flakes and ribbons [1], and recent experimental progress allows high-precision edges to be engineered [2].
Simulations play a key role in both interpreting experimental measurements and confirming the presence of desired magnetic behaviour.
However, computational costs prevent the simulation of large-scale disorders that can occur in experiment and could quench the desired behaviour.
We have developed a machine-learning approach which removes this computational bottleneck [3].
I will discuss its performance on a range of geometries, and show how spin currents in graphene nanoribbons unexpectedly survive in the presence of long-ranged edge roughness [4].

References

[1] Y.-W. Son, M. L. Cohen, and S. G. Louie, Nature 444, 347 (2006).
[2] G. Z. Magda et al, Nature 514, 608 (2014); P. Ruffieux et al, Nature (531, 489 (2016)
[3] M. E. Kucukbas, S. McCann and S. R. Power, Phys. Rev. B. 106, L081411 (2022)
[4] M. E. Kucukbas and S. R. Power, *in preparation*(2023)

Figures

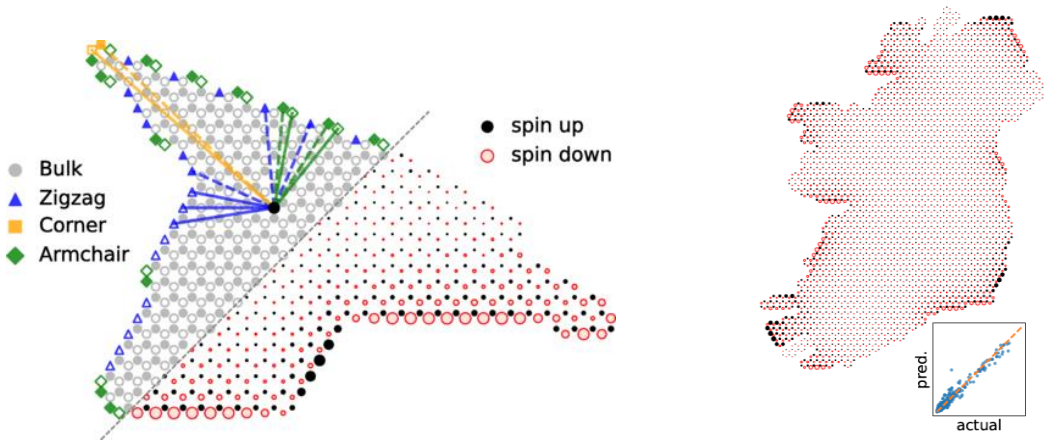

Figure 1: (Left:) Breakdown of sites in a graphene flake by sublattice, edge type and moment magnitude. (Right:) Neural network predictions of moments on an unseen geometry.