Tuning Spin Polarisation in Symmetric Graphene Nanoribbons

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Manipulating spin degrees of freedom in low-dimensional materials offers a pathway to low-energy, potentially disruptive technologies [1]. Graphene nanoribbons (GNRs), with their tuneable edge states, provide a versatile platform for exploring ways to manipulate spin [2]. However, the ground state of symmetric GNRs is an equal superposition of two Ising states (Fig. 1a), preventing the realisation of edge-based quantum spin chains. Recently, Janus GNRs (Fig. 1b), which are chemically desymmetrised GNRs, were proposed as a solution for this symmetry-breaking problem [3]. While Janus GNRs do host spin-polarised edges, their chemical asymmetry limits the possibilities of manipulating their spin states.

(a)

(b)

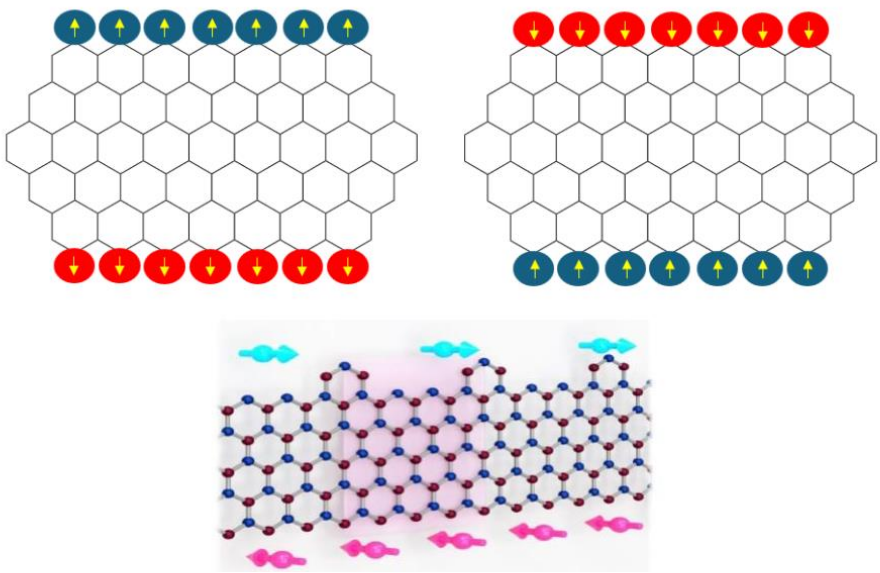

Figure 1. (a) Degenerate Ising ground states of symmetric GNRs. (b) Ground state of Janus GNRs [3].

In this work, we propose an electric field-mediated mechanism for achieving spin-polarised edges in symmetric GNRs, i.e. selecting one of the Ising states in Fig. 1a. The electric field breaks inversion symmetry by polarising the orbitals on the GNR edges [4]. In combination with spin-orbit coupling, this breaks the degeneracy of the Ising states. In contrast to Janus GNRs, using this mechanism the spin polarisation can be turned on and off using the electric field.

Our Heisenberg Hamiltonian calculations suggest that this mechanism may be achievable in symmetric GNRs with weak ferromagnetic coupling within the edge and antiferromagnetic coupling between the edges. Our molecular and periodic broken-symmetry calculations suggest that a recently synthesised GRN is a suitable candidate for testing these predictions in practice.

References:

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