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Edge defect switched dual spin filter in zigzag hexagonal boron nitride nanoribbons†

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Unlike graphene nanoribbons, zigzag monolayer hexagonal boron nitride nanoribbons (ZBNNRs) possess two distinct edges (B and N edges). Using first-principles calculations, we investigate the spin-dependent electronic transport of ZBNNRs with edge defects. It is found that the defects could make the system operate as a dual spin filter, where the direction of spin polarization is switched by the defect. Further analysis shows that the transmission eigenchannels for the opposite spins reside spatially separated on opposite edges. The defect on one edge could suppress the transmission for only one spin component, but preserve that for the other spin, resulting in a dual spin filter effect. This effect is found to be unaffected by the width of the ribbon and the length of the defect. Moreover, by constructing defects on both edges, the system exhibits two transmission peaks with opposite spins residing discretely on both sides of the Fermi level, suggesting that an electrically controlled dual spin filter based on ZBNNRs is also realizable. As controllable defects have been experimentally fabricated on monolayer boron nitride [T. Pham, A. L. Gibb, Z. Li, S. M. Gilbert, C. Song, S. G. Louie and A. Zettl, *Nano Lett.*, 2016, **16**, 7142–7147], our results may shed light on the development of B/N-based spintronic devices.

Introduction

Spintronics is a promising field for next-generation electronic devices.[1–6] Recently, two-dimensional (2D) structure-based spintronic applications have drawn much attention, such as with graphene.[7,8] Among them, monolayer hexagonal boron nitride (h-BN) also possesses a honeycomb structure, and shows application potential.[9–12] Integrating a 2D structure into a practical device generally needs further reduction of the dimensionality to fully utilise its geometric and physical properties. Interestingly, after cutting, zigzag monolayer h-BN nanoribbons (ZBNNRs) exhibit two distinct edges, *i.e.*, one consisting of only B atoms and the other consisting of only N atoms.[13] This is quite different from zigzag graphene nanoribbons, where both edges are constructed of C atoms.[14] In 2D systems such as graphene, zigzag edges usually make the system acquire magnetism[15–17] and exhibit interesting magnetic behaviors.[13,18] Recently, Pham *et al.*[9] have successfully fabricated controllable defects on h-BN by experiment. As is well known, besides creating edges, defects are also a useful way to modulate the electronic, and in particular the magnetic, structure in 2D systems.[19] Thus, for ZBNNRs, which possess special edges, the interplay between the edge and the defect may cause an interesting effect on the magnetic structure and spin-dependent electronic transport, which is expected to be used in spintronic devices. However, it is still unstudied.

In the present work, we report a first-principles investigation on the spin-dependent transport of ZBNNRs with edge defects. It is found that the B-edge defect could suppress the spin-up transmission, and does not affect the spin-down one. Meanwhile, the N-edge defect could suppress the spin-down transmission, and does not disturb the spin-up one. As a result, the system could operate as a dual spin filter, and the direction of the spin polarization is switched by the defect. Further analysis shows that the spacial separation of the transmission eigenchannels on the edges for opposite spins is the key mechanism behind this behaviour. Moreover, it is found that such an effect is unaffected by the width of the ribbon and the length of the defect, showing great application potential.

Methodology

The calculations were performed by a first-principles method based on density functional theory (DFT) combined with a

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