Electronic and magnetic properties of zigzag edges of molybdenum disulfide

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Monolayers of transition metal dichalcogenides, and particularly molybdenum disulfide (MoS_2), are among the most intensively studied 2D materials owing to their direct band gap, which makes them good candidates for electronic and optoelectronic applications. MoS_2 is a nonmagnetic semiconductor. However, several early theoretical studies have predicted magnetic moments localized on the edges of zigzag nanoribbons similar to the case of zigzag graphene nanoribbons. On the experimental side, recent magnetic measurements performed on zigzag MoS_2 nanoribbons demonstrate prominent ferromagnetic behavior. In view of these observations, it is important to understand the properties of edge magnetism in MoS_2 nanoribbons, especially in large systems where disorder cannot be excluded.

For systems involving a large number of atoms, tight-binding (TB) approach is a suitable alternative to *ab-initio* calculations. TB can provide a simple starting point for further inclusion of many-body electron-electron effects. By using parameters finely adjusted to DFT band structures together with local Coulomb interactions (the so-called Hubbard *U*), the magnetic properties of the MoS_2 nanoribbons have been investigated with a TB+U Hamiltonian. The calculations reveal a small domain-wall energy that indicates a weak magnetic coupling between the edge atoms, in remarkable contrast with zigzag graphene nanoribbons. By using randomly distributed Gaussian potentials, the effects of disorder on the magnetic properties have been investigated. Playing with the spatial disorder extension makes it possible to flip the orientation of the edge magnetic moments almost at will.[1]

1 Stability of edge magnetism against disorder in zigzag MoS P. Vancdó, I. Hagymàsi, P. Castenetto, and Ph. Lambin, Phys. Rev. Mater. 3 (2019) 094003.