# Effects of disorder in the electronic properties of monolayers and nanoribbons $MoS_2$

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Comprehensive research on electronic and spintronic properties of graphene and $MoS_2$ has been the focus of scientific attention for several years and still is [1,2]. An important issue, however, is the presence of defects that can influence these properties [3,4]. In the case of $MoS_2$, experiments have demonstrated that edges (1D defect) can host local magnetic moments [5]. However, the computational cost of the ab-initio DFT calculations for experimentally relevant system size is a downside. In this work, we first show that sulfur vacancies in monolayer $MoS_2$ induce gap states in the electronic band-structures. As a second contribution, we have investigated theoretically the magnetic properties for several nanometer long $MoS_2$ nanoribbons with zigzag edges using fine-tuned parameters in a tight-binding (TB)-Hubbard Hamiltonian. We could successfully reproduce the metallic state induced by the edges, compute large-scale nanoribbons and predict the spin domain-wall energy as well as study the effect of edge disorders on the magnetic properties [6]. Besides the full TB parametrization of the nanoribbon, we also described the band crossing the Fermi level with a one-dimensional linear chain model, allowing us to easily study ferromagnetic and anti-ferromagnetic configurations and giving us a useful way to study the energy cost for switching spins on various spots and scales. This model can be useful to study the stability and the properties of real size nanoribbons presenting spin defects and their applications.

References

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