Introducing 2D materials in vertical spintronic devices: Insight from first-principles

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Recent progresses in large scale manufacturing of 2D materials have paved the way to their integration in functional spintronic devices. 2D vdW heterostructures offer new means to achieve sharp interfaces with a layer-by-layer control of the functionality and high magneto resistance ratios have been predicted in 2D magnetic tunnel junctions. Yet, the experimental results available so far vary greatly depending on the integration pathways [1]. Seeking for increased performances, it has been shown that direct CVD growth of tunnel barriers improves significantly the quality of the ferromagnet-2D materials interfaces [2-4]. Following these developments, new phenomena such as the bias induced reversal of the magneto resistance were reported [5]. First-principles calculations can provide valuable insights into the magneto-transport mechanisms at play. Here, we report on the subtle interplay between the interface structure and the magneto-resistive behaviour of graphene and *h*-BN based MTJs [5]. We also investigate the potential of FM/transition-metal dichalcogenides (TMDCs) junctions [6], and we propose a band filtering mechanism to explain their spin properties [7].

References

[1] M. Piquemal-Banci *et al*., J. Phys. D. Appl. Phys. (2017), 50, 203002
[2] S. Caneva *et al.*, Nano Lett. (2016), 16, 1250.
[3] M.-B. Martin *et al*., Appl. Phys. Lett. (2015), 107, 012408.
[4] S. Caneva et al., ACS Appl. Mater. Interfaces (2017), 9, 29973.
[5] M. Piquemal-Banci *et al*., ACS nano (2018) 12, 4712.
[6] M. Galbiati, et al., Phys. Rev. Applied (2019) 12, 044022.
[7] V. Zatko, et al., ACS nano (2019) 13, 14468.