

# Two-Dimensional Magnetic Tunnel Junctions: Insights from first-principles

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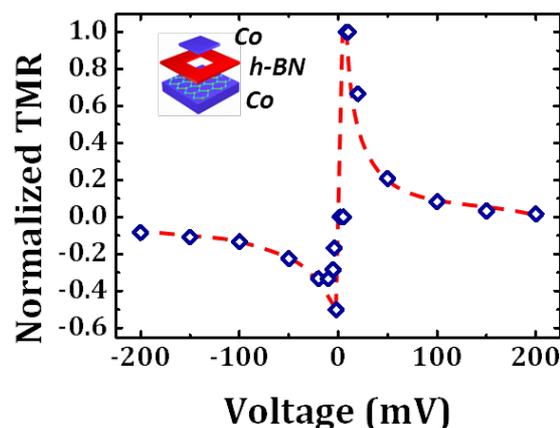
## Abstract

Two-dimensional materials are promising candidates for use as tunnel barrier in atomically thin magnetic tunnel junctions (MTJs) [1]. High magneto resistance ratios have been predicted theoretically and recent progress in large scale manufacturing of these materials has paved the way to their integrations in functional devices. Yet, the experimental results available so far vary greatly depending on the integration pathways. Seeking for increased performances, it has been shown lately that direct CVD growth of tunnel barriers improves significantly the quality of the ferromagnet-2D materials interfaces [2-4]. Following these recent developments, new phenomena such as the bias induced reversal of the magneto resistance were reported [5]. Here, we show that first-principles calculations can provide direct insights into the close relation that links the interface morphology to its magneto resistive behaviour. In particular, we reports on the origin of TMR reversal in *h*-BN based MTJs with cobalt electrodes [5].

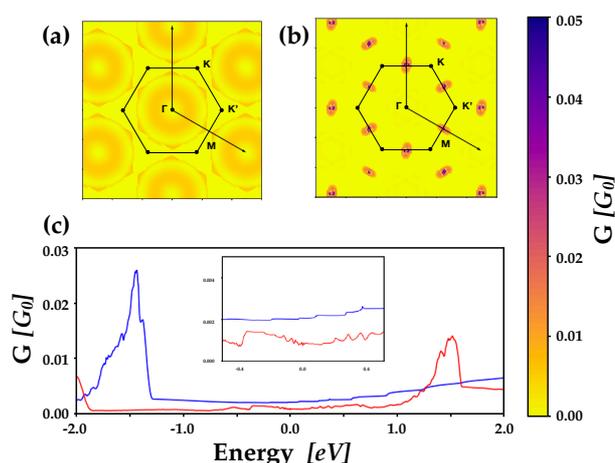
## References

- [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.
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## Figures



**Figure 1:** TMR behaviour as a function of the voltage for a Co/h-BN/h-BN/Co MTJs [5]. The blue dots are experimental data points and the red dashed lines are meant as a guide to the eye.



**Figure 2:** Origin of the spin polarization at the Co/h-BN interface. (a & b) k-resolved conductance at Fermi level for the up and down spin channels in the first Brillouin zone. (c) Total conductance of the up and down spin channels as a function of the carrier energy.