Enhancement of local Spin-Orbit Coupling effects in TMDC's/graphene heterostructures mediated by disorder

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In recent years, there is considerable interest in understanding the electronic and transport properties of graphene-based heterostructures. In particular, the heterostructure formed by graphene and two-dimensional transition metal dichalcogenides(TMDC's) is currently under extensive research [1] due to recent measurements of the Spin Hall Effect [2], and the discovery of a giant spin lifetime anisotropy [3]. However, the effects of disorder in these heterostructures is still lacking, mostly due to the high dimensionality of the systems arising from the two incommensurate lattices conforming it. In this work, we use the very recent implementation of the spin-orbit coupling of the SIESTA package [4] deployed in a high-performance computing environment, for showing the effect of disorder in the spin-texture of graphene/TMDC's heterostructures. As our main result, we found that localized defects produced a local modification of the spin-orbit coupling which can be used to increase and tune spin-orbit related phenomena as the spin Hall effect.

References

[1] Jose H. Garcia et al, Chem. Soc. Rev., 2018,47, pp 3359-3379.
[2] C. J. Safeer et al, Nano Lett., 2019, 19 (2), pp 1074–1082.
[3] Talieh S. Ghiasi et al, Nano Lett., 2017, 17 (12), pp 7528–7532.
[4] José M Soler et al 2002 J. Phys.: Condens. Matter 14 2745.

Figures

Figure 1: Bilayer supercell for TMDC/graphene heterostructure.

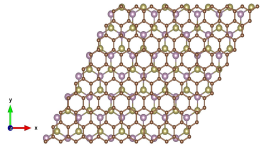

Figure 2: Electronic Band structure for WSe2 and WS2 with a vacancy in the TMDC.