

Manipulation of Spin Transport in Graphene/Transition Metal Dichalcogenide Heterobilayers upon Twisting

Jose H. Garcia

A. Pezo^{1,2}, Z. Zanolli^{3,2}, N. Wittemeier², P. Ordejón², A. Fazio^{1,4}, S. Roche^{2,5} and Jose H. Garcia²

¹Center of Natural and Human Sciences, Federal University of ABC, Brazil. ²Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain.

³Dept. of Chemistry, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands. ⁴Brazilian Nanotechnology National Laboratory/CNPEM, Brazil. ⁵Institució Catalana de Recerca i Estudis Avançats (ICREA), Spain

josehugo.garcia@icn2.cat

Proximity effects between layered materials trigger a plethora of novel and exotic quantum transport phenomena. Besides, the capability to modulate the nature and strength of proximity effects by changing crystalline and interfacial symmetries offers a vast playground to optimize physical properties of relevance for innovative applications. In this work, we use large-scale first principles calculations to demonstrate that strain and twist-angle strongly vary the spin-orbit coupling (SOC) in graphene/transition metal dichalcogenide heterobilayers. Such a change results in a modulation of the spin relaxation times by up to two orders of magnitude. Additionally, the relative strengths of valley-Zeeman and Rashba SOC can be tailored upon twisting, which can turn the system into an ideal Dirac-Rashba regime or generate transitions between topological states of matter. These results shed new light on the debated variability of SOC and clarify how lattice deformations can be used as a knob to control spin transport. Our outcomes also suggest complex spin transport in polycrystalline materials, due to the random variation of grain orientation, which could reflect in large spatial fluctuations of SOC fields.

References

- [1] Armando Pezo et al, 2D Materials, **9**, 015008M (2022)

Figures

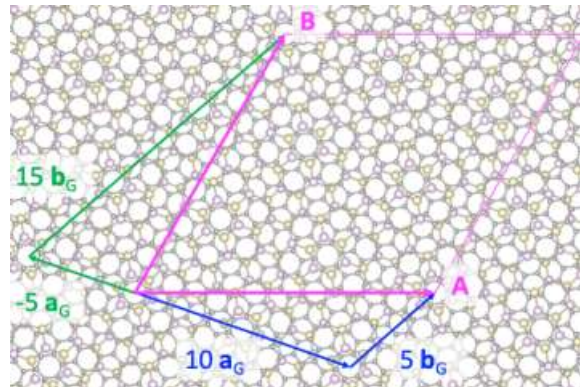


Figure 1: The Moiré periodic cell of graphene-on-MoTe₂, twisted by 30.00°. We use linear combinations of the primitive lattice vectors of graphene \mathbf{a}_G , \mathbf{b}_G to write the moiré lattice vectors $\mathbf{A} = 10\mathbf{a}_G + 5\mathbf{b}_G$, $\mathbf{B} = -5\mathbf{a}_G + 15\mathbf{b}_G$