Twist-angle dependent proximity induced spin-orbit coupling in graphene/transition-metal dichalcogenide heterostructures

Thomas Naimer
Klaus Zollner, Martin Gmitra*, Jaroslav Fabian
Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany
**Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia*
Thomas.Naimer@ur.de

We investigate the proximity-induced spin-orbit coupling in heterostructures of twisted graphene and monolayers of transition-metal dichalcogenides (TMDCs) MoS_2, WS_2, $MoSe_2$, and WSe_2 from first principles [1]. We identify strain, which is necessary to define commensurate supercells, as the key factor affecting the band offsets and thus magnitudes of the proximity couplings. We establish that for biaxially strained graphene the band offsets between the Dirac point and conduction (valence) TMDC bands vary linearly with strain, regardless of the twist angle. This relation allows to identify the apparent zero-strain band offsets and find a compensating transverse electric field correcting for the strain. The resulting corrected band structure is then fitted around the Dirac point to an established spin-orbit Hamiltonian. This procedure yields the dominant, valley-Zeeman and Rashba spin-orbit couplings. The magnitudes of these couplings do not vary much with the twist angle, although the valley-Zeeman coupling vanishes for 30° and Mo-based heterostructures exhibit a maximum of the coupling at around 20°. The maximum for W-based stacks is at 0°. The Rashba coupling is in general weaker than the valley-Zeeman coupling, except at angles close to 30°. This work was funded by the International Doctorate Program Topological Insulators of the Elite Network of Bavaria, the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) SFB 1277 (Project-ID 314695032), SPP 2244 (project no. 443416183), and by the European Union Horizon 2020 Research and Innovation Program under contract number 881603 (Graphene Flagship). M.G. acknowledges VEGA 1/0105/20.

References

[1] Naimer et al., 2021, arXiv:2108.06126 [cond-mat.mes-hall]

Figures

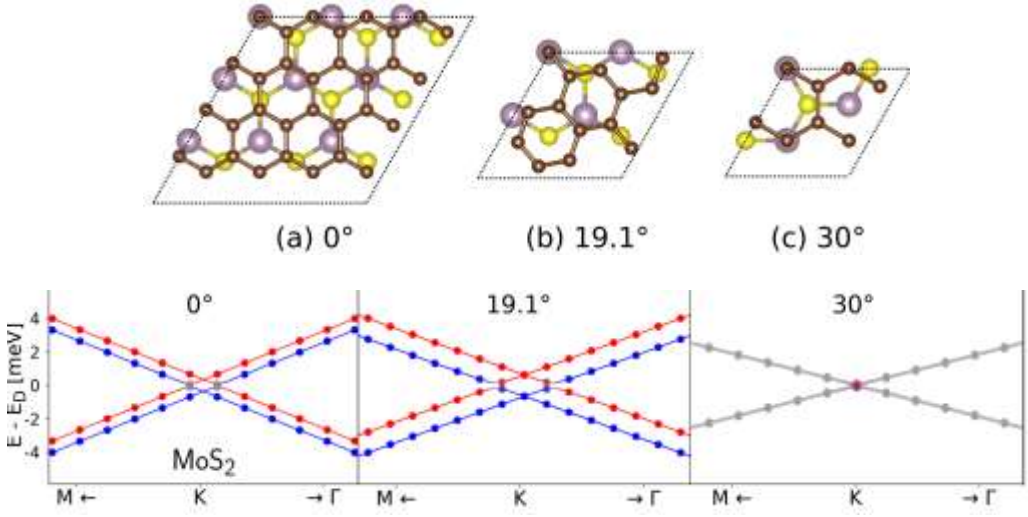

Figure 1: Unit cells and Dirac cones of MoS_2/graphene heterostructures with three different angles.