Twist-angle dependent proximity induced spin-orbit coupling in graphene/transition-metal dichalcogenide and graphene/topological insulator 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 twisted heterostructures of graphene/transition-metal dichalcogenides (MoS_2, WS_2, $MoSe_2$, and WSe_2) [1] as well as graphene/topological insulators (Bi_2Se_3 and Bi_2Te_3) from first principles. The strain in graphene, which is necessary to define commensurate supercells, is identified 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 the substrate 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, yielding the twist angle dependencies of the (Rashba and valley-Zeeman) spin-orbit coupling. This work was funded by the Elite Network of Bavaria, the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), SFB 1277, SPP 2244 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, Phys. Rev. B **2021,** 104, 195156

Figures

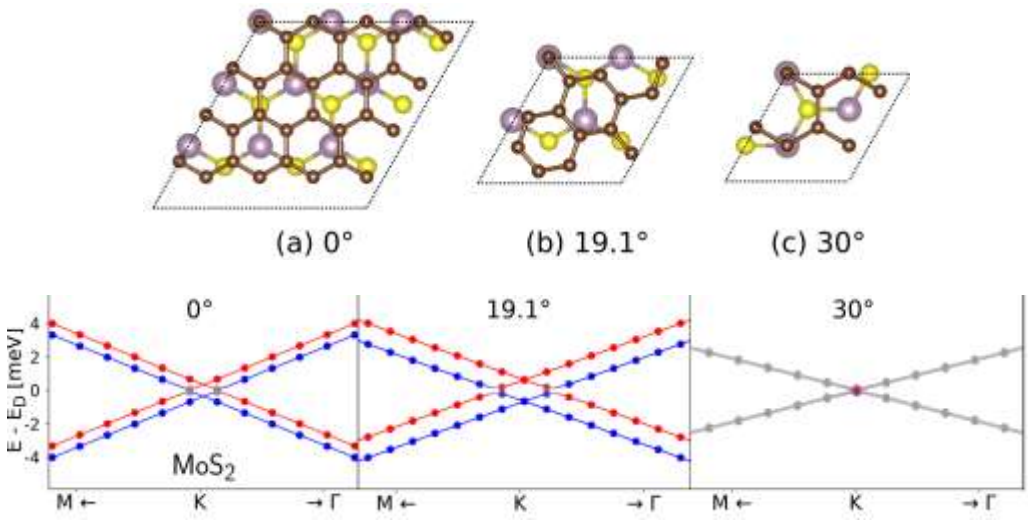

Figure 1: Unit cells and Dirac cones of MoS_2/graphene heterostructures with three different angles.