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

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Proximity effects between two-dimensional materials are giving rise to a plethora of exotic transport phenomena, with potential future disruptive applications. However, an essential issue is to properly describe their weak layer-to-layer interaction, which is strongly dependent on their relative crystalline and interfacial symmetries. Here by using large-scale first principles calculations, we found that strain and twist-angle strongly modulate the spin-orbit coupling in graphene/transition metal dichalcogenide heterobilayers, which results in giant modulation of spin relaxation times, by up to two orders of magnitude for twist-angle of 30 degrees. Additionally, the relative strengths of valley-Zeeman and Rashba spin-orbit coupling can be tailored upon twisting, which allows turning the system into an ideal Dirac-Rashba regime and generate topological transitions. These results shed new light on the debated variability of spin-orbit coupling and evidence an unprecedented possibility of spin transport control by structural deformations. This also suggests complex spin transport in polycrystalline materials, due to the random variation of grain orientation, which could reflect in large spatial fluctuations of spin–orbit coupling fields.

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Figure 1: Projected band structure of graphene on monolayer MoTe2 at zero twist angle. The gray scale indicates the projection of the band-states into carbon orbitals.

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Figures