Proximity effects in graphene/1T-TaS_2 heterostructure triggered by charge density wave and controlled with electric field

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Van der Waals heterostructures of graphene with transition metal dichalcogenides constitute highly promising systems for studies of proximity effects in graphene and their further applications in spintronics [1]. These effects include, in particular, the possibility to boost spin-orbit coupling (SOC) in graphene. In heterostructure systems, any additional degree of freedom enabling the control of proximity-induced effects is highly desirable. Such a tuning knob can be provided by charge density wave (CDW) ordering which emerges at low temperatures in selected transition metal dichalcogenides. In particular, 1T-TaS_2 develops such CDW ordering and, in addition, is predicted to acquire magnetic polarization.

In the paper, we discuss the van der Waals heterostructure composed of monolayer graphene and monolayer 1T-TaS_2 [2]. We present first-principles Density Functional Theory (DFT) calculations of its electronic structure both in the normal phase and in the CDW phase in TaS_2. Focusing on the graphene electronic structure close to the K/K' points, we predict the emergence of significant proximity effects. In order to interpret them we construct a symmetry-based tight-binding model Hamiltonian and determine its parameters by fitting the DFT data. We predict the appearence of proximity-induced Rasba and intrinsic SOC as well as exchange coupling when magnetism emerges in TaS_2 monolayer.

We find that the presence of CDW in TaS_2 profoundly influences the proximity-induced SOC in graphene, especially the Rashba SOC, modifying both its energy and Rashba angle. In this way, the CDW degree of freedom, reversibly controllable with factors such as temperature or laser light, is able to play the role analogous to the variable twist angle between the heterostructure layers, paving the way to the realization of twistronic functionalities without physically modifying a twist angle.

To add yet another tuning knob, we study the effect of the electric field normal to the heterostructure, finding the additional possibility of controlling the proximity effects.

References:

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