Proximity-induced spin-orbit and exchange coupling in graphene/1T-TaS_2 van der Waals heterostructure controlled with charge density wave and electric field

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Among various functionalities, van der Waals heterostructures offer twistronic degree of freedom, which allows design of their electronic structure. Owing to proximity effects occurring in such systems, diverse physical phenomena can be explored, maximizing the potential for applications in modern spintronics. A highly promising class of heterostructures is constituted by monolayer transition metal dichalcogenides (TMDCs) combined with graphene [1]. Particularly interesting member of TMDCs group exhibiting outstanding properties is 1T-TaS_2, as it develops a low-temperature charge density wave (CDW) phase profoundly changing the electronic properties compared to its normal phase [2].

In the paper we discuss the first-principles DFT/DFT+U calculations of the electronics properties of 1T-TaS_2/graphene heterostructure with top and hollow stacking, aimed at description of the proximity-modified band structure of graphene [3]. We develop and parametrize a symmetry-based tight-binding Hamiltonian, capable of reproducing well the DFT results for normal and CDW phase. In particular, we predict the substantial influence of the emergence of CDW on the Hamiltonian parameters, making CDW a convenient tuning knob useful to control the proximity effects in a way implementing twistronics without physical change of layers twist. The CDW degree of freedom can be reversibly controlled by thermal, optical or electric means. The proximity-induced terms include Rashba spin-orbit coupling with variable magnitude and Rashba angle, yielding tilted in-plane spin pattern; tuning of the mentioned parameters may be crucial for achieving efficient spin-charge conversion [4,5]. In addition, monolayer 1T-TaS_2 is predicted to develop an in-plane magnetic polarization, constituting another source of controllable exchange effects in graphene, superimposing on the CDW fingerprint. Moreover, we demonstrate that auxiliary factor shaping the electronic structure and tuning the spin-orbit coupling parameters is perpendicular electric field, influencing the charge transfer occurring between graphene and underlying TMDC monolayer.

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