The Effect of External Electric Field on Electronic and Spin Properties of MoS_2-graphene van der Waals Heterostructures

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Due to its exceptional electrical, optical, and spin properties, two-dimensional (2D) material is one of the most fascinating topics. The most well-known 2D material, graphene, offers a wide range of potential uses in spintronics, and electrical devices. Transitional-metal dichalcogenides (TMDs) have received a lot of attention following the discovery of graphene because they exhibit direct band gaps that match to the visible light spectrum, indicating the possibility of optoelectronic device applications[1]. Understanding the electronic properties and how to control them become one crucial aspect to creating such new devices, addressing the significance of optoelectronic application. As of now, it has been discovered that introducing an electric field is a great approach for adjusting the electronic properties of heterostructures. This method has been used successfully by several prior studies since it is beneficial. In this study, by using first-principles calculations, we provide a comprehensive analysis of the electrical characteristics of MoS_2/graphene van der Waals heterostructures and pay particular emphasis to spin-related characteristics including spin Hall conductivity. The computations were performed utilizing the generalized gradient approximation (GGA) as the exchange-correlation and the full-potential augmented plane wave (FLAPW) approach. The heterostructures of MoS_2/graphene is formed of 1×1 in-plane lattice periodicity in the slab model, in which an external electric field applied in the vacuum regions far from both slab surfaces varies from -0.8 V/nm to +0.8 V/Å. As the result of forming the heterostructures, a small band gap opening is emerged in the MoS_2/graphene originating from symmetry breaking in the system, agreed with previous calculations [2]. Applying external electric field along +z and -z direction has a different effect on the band gap of MoS_2/graphene heterostructures. A larger external electric field increases the spin Hall conductivity of in MoS_2/graphene heterostructure. The spin Hall conductivity results show that the MoS_2/graphene is an interesting heterostructure for spin Hall conductivity properties due to the significant changes depending on the magnitude of the electric field. A comprehensive and detailed discussion of the results of electronic and spin properties of MoS_2/graphene heterostructure is presented.

References:

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