Electronic properties of MoS_2-WS_2 heterojunction

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The fabrication of electronic devices based on a single or a few layers of transition metal dichalcogenides , such as MoS_2 and WS_2, holds the promise of expanding the graphene revolution into an exciting new arena. Unlike graphene, the MoS_2 and WS_2 monolayers have a direct band gap in the 1.8eV range and, due to the strong spin orbit coupling (SOC) and the specifics of their atomic structure, they present strong spin-valley coupling. This has been demonstrated by means of optical pumping experiments which to valley polarized exciton population [1-3].

Here we study the electronic structure of a heterojunction made of two monolayers of MoS_2 and WS_2. Our first-principles density functional calculations [4] show that, unlike in the homogeneous bilayers, the heterojunction has an optically active band-gap, smaller than the ones of MoS_2 and WS_2 single layers. We find that that the optically active states of the maximum valence and minimum conduction bands are localized on opposite monolayers, and thus the lowest energy electron-holes pairs are spatially separated. Our findings portrait the MoS_2-WS_2 bilayer as a prototypical example for band-gap engineering of atomically thin two-dimensional semiconducting heterostructures.

We also find that, contrary to previous theory work, there is spin splitting at the K point both in the valence and the conduction band. We discuss the physical origin of the splitting at the conduction band and derive an effective Hamiltonian making use of Wannier functions and perturbation theory.

References:
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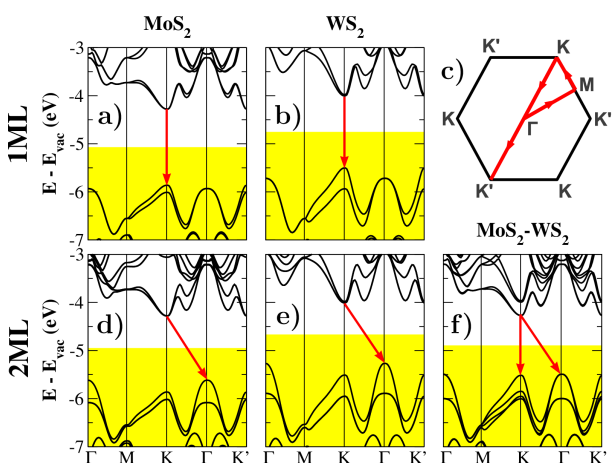

Fig.1: Band structures of (a) MoS_2 monolayer, (b) WS_2 monolayer, (d) MoS_2 bilayer, (e) WS_2 bilayer, and (f) MoS_2- WS_2 heterojunction. (c) Scheme of the Brillouin zone.