

Electronic properties of MoS₂-WS₂ bilayers

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Abstract

The fabrication of electronic devices based on a single or a few layers of transition metal dichalcogenides, such as MoS₂ and WS₂, holds the promise of expanding the graphene revolution into an exciting new arena. Unlike graphene, the MoS₂ and WS₂ 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].

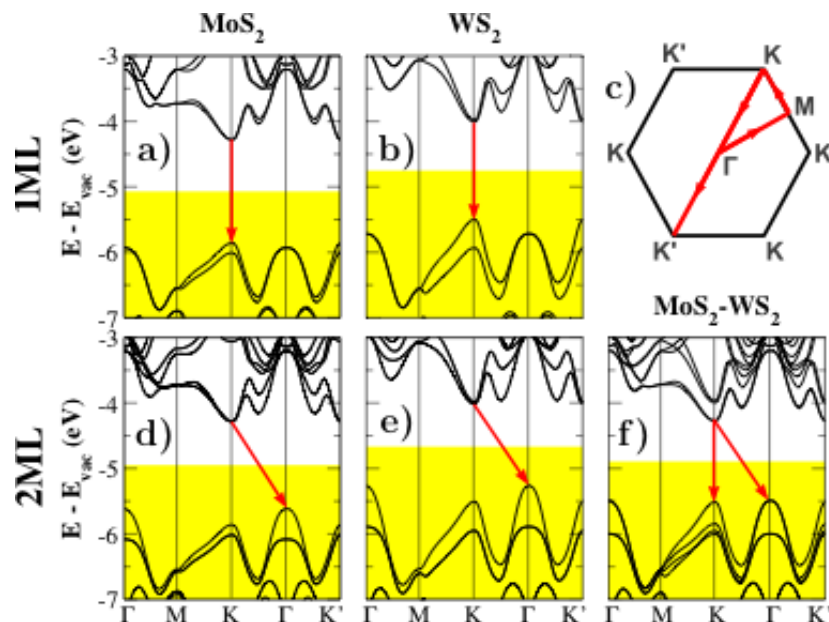
Here we study the electronic structure of a heterojunction made of two monolayers of MoS₂ and WS₂. Our first-principles density functional calculations show that[4], unlike in the homogeneous bilayers, the heterojunction has an optically active band-gap, smaller than the ones of MoS₂ and WS₂ single layers. 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 MoS₂-WS₂ 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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- [3] T. Cao, G. Wang, W. Han, H. Ye, C. Zhu, J. Shi, Q. Niu, P. Tan, E. Wang, B. Liu, and J. Feng, *Nature Communications* **3**, (2012) 887.
- [4] K. Kosmider, J. Fernández-Rossier, arXiv:1212.0111

Figures



Caption: Calculated electronic structure of MoS₂, WS₂ monolayers and bilayers, as well as the (Mo-W)₂ bilayer.