Interlayer screening in n-doped bilayer transition metal dichalcogenides

Andor Kormányos ⁽¹⁾ Viktor Zólyomi ⁽²⁾, Guido Burkard ⁽¹⁾

⁽¹⁾ University of Konstanz, Germany ⁽²⁾ Manchester University, United KIngdom

andor.kormanyos@uni-konstanz.de

The breaking of crystal symmetries can have profound effects on the electrical and optical properties of materials. Several intriguing experimental observations, such as the electrical tuning of valley magnetic moment[1], spin-layer locking[2], and valley Hall effect[3] have recently been reported in bilayers of transition metal dichalcogenides (TMDCs) and ascribed to the inversion symmetry breaking effect of an external electric field.

Motivated by these observations, we consider n-doped bilayer TMDCs placed in uniform external electric field and discuss the charge re-distribution between the layers due to the electric field. We calculate the band gap that opens at the K-point of the Brillouin zone in self-consistent Hartree approximation. We discuss the relation between the induced band-gap and the quantum capacitance and point out the difference between different stacking configurations (AB vs AA).

Finally, the relevance of our results to recent photoluminiscence experiments in double gated bilayer MoS2 [4] is briefly considered [5].

References

- [1] Wu, S. et al., Nature Physics **9**, 149 (2013).
- [2] Jones, A. M. et al., Nature Physics **10**, 130 (2014).
- [3] Lee, J., Mak, K. F., and Shan, J., Nature Nano **11** 421, (2016).
- [4] Klein, J et al., Nano Letters **16**, 1554 (2016).
- [5] Wierzbowski, J, in preparation.