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Interlayer excitons in van-der-Waals heterostructures: MoS_2 on GaSe

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Hybrid van-der-Waals heterostructures of two-dimensional nanomaterials are a vibrant field of study: The (weak) electronic interaction between two layers is often reasonably described by a perturbation of the physical effects of the isolated layers, such as electrostatic doping and increased screening of *intralayer* excitons. However, it turns out that this picture of the weak interaction is not exhaustive in terms of all optical properties: the formation of bound excitons from electrons of one layer and holes from the other layer yields the formation of *interlayer* excitons. These mixed states are measured experimentally by photoluminescence and photocurrents and predicted by theory. Examples are of MoS_2 or $MoSe_2$ on WSe_2, MoS_2 or GaSe due to type-II band alignment [1-3].
The conditions for the formation of interlayer excitons are elucidated from a first-principles point of view. For this, first-principles studies of a minimal test system of MoS_2 on GaSe is conducted [1].
This work envisions to predict the interlayer states as a function of the heterostack in order to specifically tailor efficient photon absorption.

References

[1] M. Rahaman, C. Wagner *et al.*, J. Phys.: Condens. Matter 31, 114001 (2019).
[2] H. Fang, C. Battaglia *et al.*, PNAS 111, 6198 (2014).
[3] P. Rivera, J. R. Schaibley *et al.*, Nat. Commun. 6, 6242 (2015).

Figures

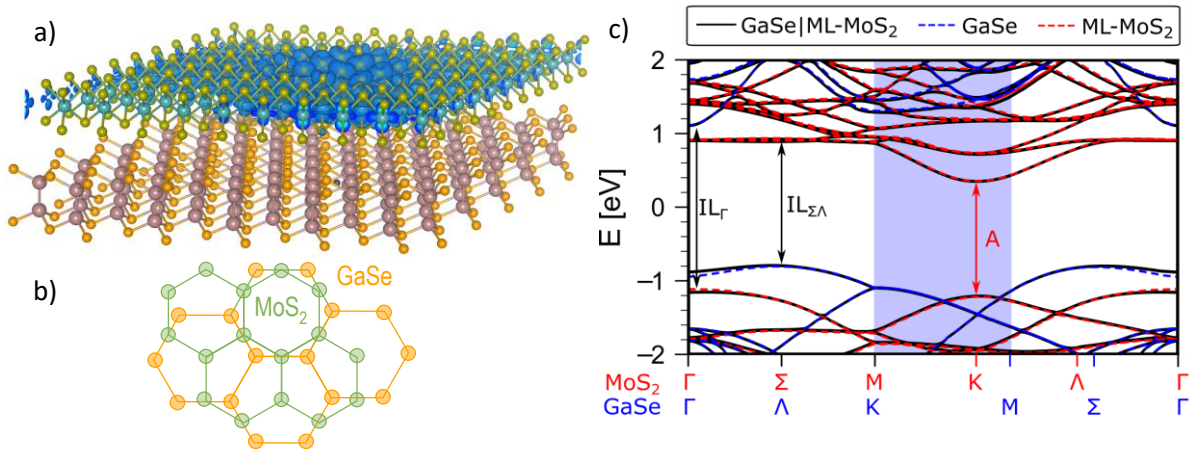

Figure 1: a) The MoS_2|GaSe bilayer and the hole exciton wave function for the interlayer exciton at Λ. b) Both materials form a nearly commensurate superlattice at a rotation angle of 30°. c) The band structure of the bilayer system compared to the band structure of the individual layers: The MoS_2 layer is polarized by the proximity of the GaSe layer. As a consequence, the conduction band edge of GaSe is higher in energy than the one of MoS_2 (type-II alignment) and additional GaSe valence band states appear within the band gaps of the pristine MoS_2.