Optical excitations in stacked van der Waals materials

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Atomically thin 2D materials have recently received huge interest due to their plethora of unique optical properties as well as the possibility to stack them into van der Waals heterostructures with superior and tailored properties.

In the first part of the presentation, I will introduce a computational database of more than 1500 2D materials with a variety of structural, elastic, electronic, magnetic, dielectric, and optical properties calculated by state-of-the-art ab-initio method.

The second part of the presentation will focus on electronic excitations in stacked van der Waals materials. They can have interlayer or intralayer character depending on the spatial localization of the involved charges (electrons and holes). In the case of neutral electron-hole pairs (excitons), both types of excitations have been explored theoretically and experimentally [1,2]. We provide a detailed picture of the most prominent excitons in bilayer MoS_2 – a prototypical van der Waals material. The lowest exciton has intralayer character and is almost independent of an electric field.
However, we find higher lying excitons that have interlayer character. They can be described as linear combinations of the intralayer exciton and optically dark charge transfer excitons. Interestingly, these mixed interlayer excitons have strong optical amplitude and can be easily tuned by a perpendicular electric field.

In contrast to neutral excitons, studies of charged trions have so far been limited to the intralayer type. In this study we investigate the complete set of interlayer excitations in an MoS_2/WS_2 heterostructure (Figure 1) using a novel ab initio method [3], which allows for a consistent treatment of both excitons and trions at the same theoretical footing. Our calculations predict the existence of bound interlayer trions below the neutral interlayer excitons. We obtain binding energies of 18/28 meV for the positive/negative interlayer trions with both electrons/holes located on the same layer. In contrast, a negligible binding energy is found for trions which have the two equally charged particles on different layers [4].

References

[1] S. Latini et al., Nano Letters 17, 938 (2017).
[2] N. R. Wilson et al., Science Advances 3, e1601832 (2017).
[3] T. Deilmann, M. Drüppel, and M. Rohlfing, PRL 116, 196804 (2016).
[4] T. Deilmann, and K.S. Thygesen, Nano Letters 18, 1460 (2018).

Figures

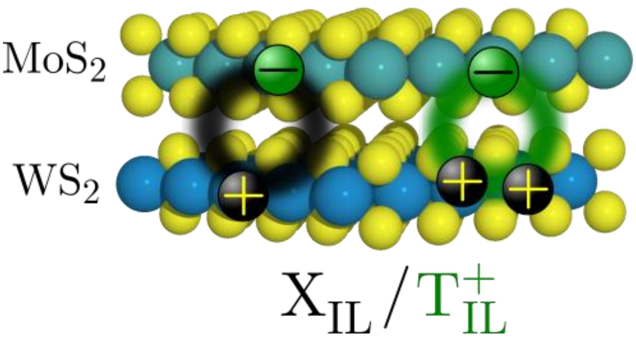

Figure 1: Interlayer exciton (black) and interlayer trion (green) in an MoS_2/WS_2 heterostructure.