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Optical properties and giant valley polarization of interlayer excitons in van der Waals heterostructures

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Abstract

The 2D materials, such as monolayer transition metal dichalcogenides (TMDs) 1-4, can form van der Waals (vdWs) heterostructures held together by weak van der Waals forces, providing an unprecedented platform to engineer quantum materials with exotic physical properties. Among the different vdWs heterostructures, the most interesting ones for optical applications are those characterized by a type II band alignment where the valence band maximum and the conduction band minimum lie in different layers. This configuration energetically promotes ultrafast charge separation, prompting the photoexcited electrons to reside on one TMD layer and the holes to be on the other, forming interlayer excitons (IXs). The IXs possess the recombination times and valley lifetimes several orders of magnitude longer than that of the monolayer excitons, making them ideally suited for some spintronics and valleytronic device applications. A weak interlayer vdW interaction, however, inhibits interlayer charge transfer across vdW heterostructures, significantly constraining the population of the IXs. In addition, the reduced oscillator strength of IXs renders them further darkish. The small population together with the darkness of the IXs substantially limit their experimental probing and potential applications. In this work, firstly, we will present our computational packet–WanTiBEXOS which is a parallel computational FORTRAN code, constituted of a maximally localized Wannier functions based tight-binding model in conjunction with the Bethe–Salpeter equation framework. Our packet can be used to study optical properties of excitons including IXs in conventional semiconductors, 2D magnetic and non-magnetic materials, TMD vdW heterostructures and perovskite, etc.. After that, we will move to magnetic proximity effect on IX dynamics in the TMD vdWs heterostructures grown on magnetic substrate5, focusing on optical properties and giant valley polarization of interlayer excitons.

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Orateur: Prof. QU, Fanyao (Universidade de Brasília)

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