Exciton and trion features in MoS_2/WS_2 heterobilayer: Theoretical study

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Abstract

In the recent years, two-dimensional (2D) materials have attracted an increasing interest due to the ability to fulfill the future demands of the nanoelectronic device and their potential applications in the next generation low-cost solar cells [1]. Monolayers of group-VI transition metal dichalcogenides (TMDs) have recently emerged as a new class of direct-gap semiconductors in the two-dimensional (2D) limit and the visible range band gap further makes these 2D semiconductors ideal platforms for optoelectronics and light-harvesting applications [2]. Stacking different TMDs monolayers to form van der Waals heterostructures opens open up venues to creating new material systems exploited at nanoscale, with rich functionalities and novel physical effects. Importantly, MX_2 heterostructures are predicted to form type II heterojunctions in which the conduction band minimum and valence band maximum reside in two separate materials giving an efficient separation of electrons and holes [3]. Very Recently, MoS_2/WS_2 heterobilayers have been realized by Sefaattin Tongay and collaborators [3] using CVD grown monolayers. They have highlighted that the PL spectrum of the herein heterobilayers changes versus annealing time, from additive PL to renormalized one. This is manifested in the PL spectrum by the appearance of multiple-peak and gradual reduction of others. These peaks correspond to neutral and charged exciton coming from the constituent monolayers. To provide an insight on the observed phenomena, we suggest a theoretical investigation based on two and three-body Hamiltonian, in which the electron-hole interaction is taken in consideration. To propose the key parameters for the analytical model, we have carried out Density Functional Theory (DFT) calculations [4] on the monolayers MoS_2, WS_2 and the present heterostructure. We have elucidated the corresponding electronic structure including the bands structure, angular momentum contribution and effective masses of charge carriers. We have also determined several significant optical properties, in particular, the dielectric constants of the herein materials.

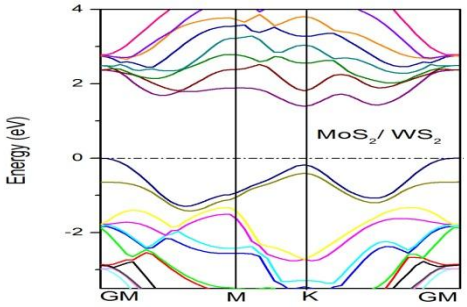

Figure.1. Bands structure of MoS_2/WS_2 heterobilayers

References

[1] C. C. Neto and K. S. Novoselov, Mater. Express **1**, 10 (2011).

[2] A. Splendiani et al, Nano Lett **10,** 127 (2010).

[3] S. Tongay et al Nano Lett.**14**, 3185 (2014).

[4] P. Hohenberg and W. Kohn Phys. Rev B.**136**, 864(1964).