Binding energies of exciton complexes in two-dimensional transition metal dichalcogenide

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Abstract

Excitonic effects play an important role on the optoelectronic behavior of atomically thin two-dimensional crystals of the tungsten transition metal dichalcogenide (TMD). Neutral and charged exciton behaviors in monolayer (ML) TMD are handled within effective-mass approximation in which the critical parameters are ensured from our ab-initio calculations. Firstly, we reveal an exciton series with a novel energy dependence on the orbital angular momentum. We show that, states corresponding to higher angular momentum have a larger binding energy than those corresponding to lower angular momentum. We either demonstrate that the trion with two heavier identical carriers has a larger binding energy [1]. Considerable control of the dielectric environment on exciton binding energy is elucidated in Fig.1. Secondly, we use the equilibrium mass action law, to quantify the relative weight of exciton and trion PL. We show that exciton and trion emission can be tuned and controlled by external parameters like temperature, pumping and injection electrons [2]. Thirdly, localization of neutral exciton center of mass motion arising from ML defect has been also studied (Fig.2). Our obtained results are in agreement with available experimental works [3].

References

[1] A. Hichri, I. Ben Amara, S. Ayari and S. Jaziri, Journal of Physics Condensed Matter, 29 (2017) 435305.
[2] A. Hichri, I. Ben Amara, S. Ayari and S. Jaziri, Journal of Applied Physics, 121(2017) 235702.
[3] B. Zhu, X. Chen and X. Cui, Sci. Rep., 5 (2015) 9218.

Figures

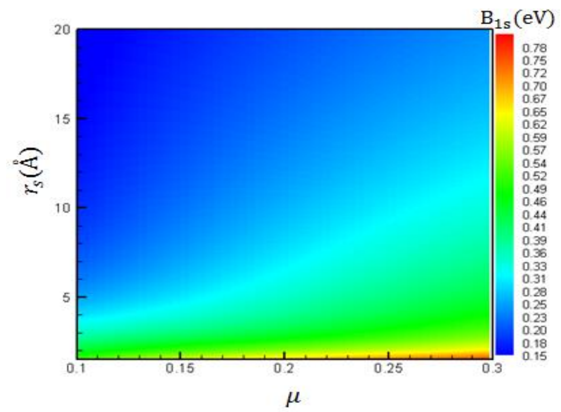

Figure 1: Color surface plot of the exciton binding energy B_{1s} in ML WS_2. Calculations are performed over a range of material screening lengths rs and possible exciton reduced masses μ. The average dielectric constant of the surrounding material is $\kappa = 2.5$.

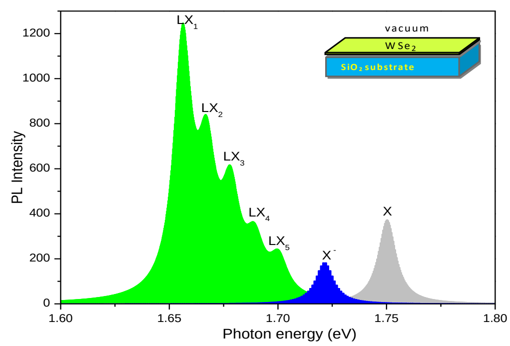

Figure 2: One-photon PL spectrum for free, localized exciton and trion in ML WSe_2 at a temperature of T=10 K. The spectrum shows five pronounced PL peaks, which are located between 1.62-1.72 eV. The emission from the neutral and charged exciton is substantially reduced in the presence of localized states.