20th Brazilian Workshop on Semiconductor Physics

Tunable properties of excitons in double monolayer heterostructures

Luiz G. M. Tenório[1,2], **Teldo A S Pereira**[1], Kamyar Mohseni[2], Tobias Frederico[2], Mohammadreza Hadizadeh[3,4], *Diego Rabelo da Costa*[5], *André J. Chaves*[2]

[1] *Instituto de Física, Universidade Federal de Mato Grosso, 78060-900, Cuiabá, Mato Grosso, Brasil*
[2] *Departamento de Física, Instituto Tecnológico de Aeronáutica, DCTA, 12228-900 São José dos Campos, Brasil*
[3] *College of Engineering, Science, Tech. and Agriculture, Central State University, Wilberforce, OH, 45384, USA*
[4] *Department of Physics and Astronomy, Ohio University, Athens, OH, 45701, USA*
[5] *Departamento de Física, Universidade Federal do Ceará, Campus do Pici, 60455-900 Fortaleza, Ceará, Brazil*

teldo@fisica.ufmt.br

Abstract

Nowadays, the so-called van der Waals heterostructures represent a prominent research area within optoelectronics in semiconductor 2D materials. The layered structures are related to the fact that they support the formation of excitons – bound electron-hole pairs – and excitonic complexes with binding energies more than an order of magnitude greater than conventional semiconductors, i.e. on the order of hundreds of meV, and small Bohr radii in the range of several nanometers[1-6]. In this work, we study the exciton properties of double layers of transition metal dichalcogenides (TMDs), where between the layers we have a dielectric spacer. We used an expansion of Chebyshev polynomials to solve the Wannier equation for the exciton. We systematically study both homo and hetero double layer systems for MX_2, showing the dependence of the inter and intralayer excitons binding energy as functions of the spacer width and dielectric constant. We also show how the exciton energy, that includes the effects of the changing band gap, depends on those geometric properties.

References

[1] T. C. Berkelbach, M. S. Hybertsen, and D. R. Reichman, Physical Review B **88**, 045318 (2013).
[2] C. Zhang, A. Johnson, C.-L. Hsu, L.-J. Li, and C.-K. Shih, Nano letters **14**, 2443 (2014).
[3] K. He, N. Kumar, L. Zhao, Z. Wang, K. F. Mak, H. Zhao, and J. Shan, Physical review letters **113**, 026803 (2014).
[4] Z. Ye, T. Cao, K. O'brien, H. Zhu, X. Yin, Y. Wang, S. G. Louie, and X. Zhang, Nature **513**, 214 (2014).
[5] M. M. Ugeda, A. J. Bradley, S.-F. Shi, H. Felipe, Y. Zhang, D. Y. Qiu, W. Ruan, S.-K. Mo, Z. Hussain, Z.-X. Shen, et al., Nature materials **13**, 1091 (2014).
[6] T. Cheiwchanchamnangij and W. R. Lambrecht, Physical Review B **85**, 205302 (2012).

Figures

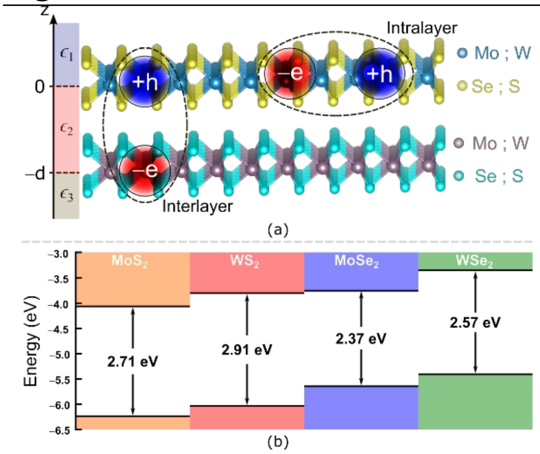

Figure 1:. a) Schematic illustration of the double layered TMDs, separated by a spacer of dielectric constant ϵ_2 $(-d \leq z \leq 0)$ and width d, immersed in two materials of dielectric constants ϵ_1 $(z > 0)$ and ϵ_3 $(z < -d)$. This structure sustains both intralayer and interlayer excitons. (b) band alignment as measured from vacuum between the four TMDs considered in this work.