Electronic properties studies of transition-metal dichalcogenides quantum dots

L. Szulakowska [1], P. Potasz [1] and A. Wójs [1]

[1] *Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, Wrocław, Poland*

We study the electronic structure of quantum dots of group-VIB transition metal dichalcogenides MX2 (M: Mo, W and X: S, Se, Te) [1]. Their honeycomb lattice, analogous to graphene, has importantly distinct properties to graphene. In MX2 monolayers inversion symmetry is explicitly broken, which gives rise to valley-dependent optical selection rules for interband transitions at K points of hexagonal BZ. Moreover, transition-metal dichalcogenides exhibit strong spin-orbit coupling, which results in a large valence-band spin splitting at the K point [2].

We investigate electronic properties of finite size fragments of transition-metal dichalcogenides and compare their properties to graphene quantum dots [3,4]. The electronic structure of the quantum dots is obtained within three-band TB model with the nearest-neighbours and the next nearest neighbours hoppings included [5]. We investigate nanostructures of different shapes, sizes, and edge types. The geometry of the quantum dots is optimized within density functional theory (DFT) methods. The process of edge relaxation and its effect on the electronic properties of the nanostructures is also studied. The effect of spin-orbit coupling is analyzed.

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