Theory of electronic structure of monolayer and nanostructured MoS_2 and role of electron-electron interactions on its optical properties

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In the following work minimal, graphene-like tight binding model of single layer of transition metal dichalcogenide (TMDC) MoS_2 is derived [1]. There is currently renewed interest in understanding the electronic and optical properties of TMDCs with formula MX_2 (M, metal from group IV to VI; X = S, Se, Te). A tight-binding model which illuminates roles of metal-chalcogen and metal-metal interactions, allows for inclusion of magnetic field, confinement, and many-body interactions is desirable. We start our analysis from identifying the most important orbitals for the low energy physics, basing our choice on symmetry arguments and first-principles calculations. Next, we analyse contribution of nearest- and next- nearest neighbour interaction effects to the band structure around Fermi level. Then we derive Landé, valley Zeeman and Landau g-factors, illuminating role of p orbitals in their values. Spin-orbit interaction is also derived and spin textures of valence and conduction bands are discussed. In second part theory of nanostructures is presented for quasi one – dimensional and zero – dimensional systems. Properties of edge states in zigzag and armchair nanoribbons are analysed. Then, properties of MoS2 quantum dots are studied, paying special attention to the role of edge states. In last part we construct effective theory of optical response of this material, which is dominated by neutral and charged excitons. We analyse effects of interactions of optically created electron and hole pairs with other electrons in valence band, and then using Bethe-Salpeter equation we obtain simplest properties of bound electron-hole state. Qualitative properties of charged excitons are also discussed. We conclude by discussing role of interactions screening on the abovementioned effects.

References

[1] M. Bieniek, M. Korkusiński, L. Szulakowska, P. Potasz, I. Ozfidan, and P. Hawrylak, „Band nesting, massive Dirac fermions, and valley Landé and Zeeman effects in transition metal dichalcogenides: A tight-binding model", Phys. Rev. B 97, 085153 (2018).