Band nesting and valley exciton in monolayer MoS₂ M. Bieniek^{1,2}, L. Szulakowska² and P. Hawrylak²

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We report the effect of band nesting on single valley excitons in monolayer MoS_2 . We start with ab-initio based electronic structure obtained within tight binding model of MoS_2 [1]. We next turn on electron-electron interactions, form a Hartree-Fock ground state and construct electron-hole excitations. We compute e.-e. interactions, self-energy in the screened exchange and Coulomb hole approximation and direct and exchange electron-hole interaction. We solve Bethe-Salpeter equation to obtain exciton states and absorption spectrum. We disentangle effects of electron-hole dispersion, details of band structure on Coulomb intra/inter - valley interactions, topology, screening and dielectric environment. In particular, we discuss the effect of Q-points and band nesting on ground and excited states of excitons in MoS_2 .

[1] M. Bieniek, M. Korkusiński, L. Szulakowska, P. Potasz, I. Ozfidan, and P. Hawrylak, PRB 97, 085153 (2018).