

# Fine structure of neutral and charged excitons in monolayer MX<sub>2</sub> TMDs

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We report here the effect of band nesting and topology on fine structure of excitons and trions in monolayer transition metal dichalcogenides (TMDs) family of 2D semiconductors [1]. We start with ab-initio based electronic structure obtained within tight-binding model of family of MX<sub>2</sub> (M=Mo,W, X=S,Se,Te) direct gap semiconductors [2]. We next turn on electron-electron interactions, form a Hartree-Fock ground state and construct electron-hole excitations. We compute electron-electron interactions, i.e. direct and exchange electron-hole interaction. We solve Bethe-Salpeter equation to obtain highly converged spectrum of exciton states. We disentangle effects of electron-hole dispersion, details of band structure on Coulomb intra/inter - valley interactions, topology of wavefunctions, screening and dielectric environment. In particular, we discuss the effect of SU(3) symmetric Q-points and band nesting on ground and excited states of excitons. By precise inclusion of spin splitting in our calculations, we establish splitting between dark and bright exciton species. Next, motivated by recent experiments [3], we propose novel intra- and inter-valley singlet trions, constituting the trion fine structure distinct from that already known in bright and dark 2D materials with large conduction-band splitting induced by the spin-orbit coupling. We show that the trion energy splitting in MX<sub>2</sub> is a sensitive probe of inter- and intra-valley carrier interaction.

[1] [M. Bieniek](#), L. Szulakowska, and P. Hawrylak, „Band nesting and exciton spectrum in monolayer MoS<sub>2</sub>”, *Phys. Rev. B* 101, 125423 (2020).

[2] [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).

[3] J. Jadcak, J. Kutrowska-Girzycka, [M. Bieniek](#), T. Kazimierczuk, P. Kossacki, K. Watanabe, T. Taniguchi, C.-H. Ho, A. Wójs, P. Hawrylak, and L. Bryja, “Fine structure of charged and neutral excitons in monolayer MoS<sub>2</sub>”, *Nanotechnology* 32 (14), 145717, (2021)