Optical investigations of dark and bright three-particle states in 2D semiconductors

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2D transition metal dichalcogenides (TMDCs) of the type MX_2 (M = Mo, W; X = S, Se, Te) have recently revealed exciting physical phenomena, offering unique functionalities relevant for future applications in valleytronics and quantum technologies. Coulomb-bound two-particle states known as excitons play a central role in the optical response of these materials. Their binding energies exceed those of conventional III-V semiconductors such as GaAs by one to two orders of magnitude, providing an ideal platform to study these neutral or charged quasiparticles and their excited states at elevated temperatures.

We reveal the importance of dark and bright Coulomb-bound three-particle states in monolayer crystals of MoS_2, $MoSe_2$, WS_2 and WSe_2 encapsulated between thin layers of hBN [1,2]. Using optical absorption and photoluminescence (PL) spectroscopy combined with *GW*-BSE *ab initio* calculations, we find that the lowest energy trions in WS_2 and WSe_2 monolayers are optically 'dark' [1]. For $MoSe_2$, the ground-state trion is optically 'bright', while it is a mixed bright-dark state in MoS_2 monolayers [1]. This has pronounced effects on their optical emission and absorption properties at different temperatures. We also show that the excited state (2s) of a trion (Fig.1) is present in a WS_2 monolayer [2].

Our results underline the importance of trions in the entire excitation spectrum of atomically thin semiconductors, and are important for future trion-based valleytronic devices [3].

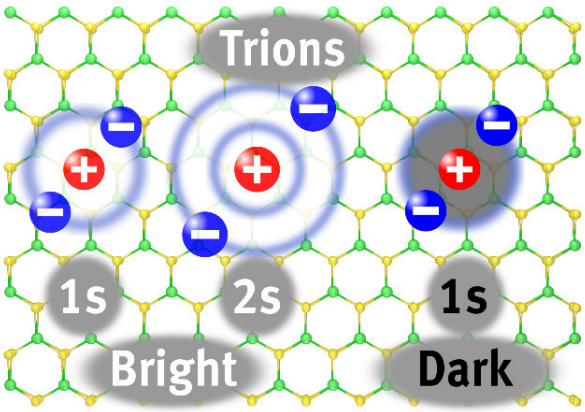

Figure 1: Schematic drawing of ground (1s) and excited (2s) states of a trion in a 2D semiconductor.

References

[1] A. Arora et al., Phys. Rev. B **101**, 241413 (2020) [Dark trions in TMDCs]
[2] A. Arora et al., Phys. Rev. Lett. **123**, 167401 (2019) [Excited-state trions in TMDCs]
[3] A. Arora et al., J. Appl. Phys. **129**, 120902 (2021) [Invited perspective on TMDC research]