Upconversion photoluminescence of a defect-bound exciton in hBN- encapsulated MoS_2 monolayers

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Recent advances in the elaboration of high-quality TMDCs monolayers surrounded by hBN have provided in-depth insights into the excitonic complexes properties as well as the exciton-exciton and exciton-phonon interactions revealed by optical spectroscopy experiments [1]. However, TMDCs monolayers prepared by mechanical exfoliation can have a native defect density of about 10^{13} cm^{-2} [2], which usually reduces the performance of their opto-electronic properties. These atomic defects mainly comprise chalcogen vacancies, which can form gap states and alter doping. Hence, in most TMDCs monolayers the broad sub-gap emission appears at low temperatures about several hundred meV below the neutral exciton X. This sub-gap luminescence is often called L-band and typically its intensity grows for increasing density of point defects and can be observed over a wide range of temperatures, even up to room temperatures [3].

Here, we demonstrate upconversion (UPC) photoluminescence (PL) of a defect-localized exciton X_L in hBN/MoS_2/hBN structures with a high energy gain of about 292 meV at 7 K. The upconverted PL is observed only for samples in which the prominent X_L line dominates the neutral exciton X in low-temperature PL spectra. Furthermore, we evaluate the UPC PL dependence on changes in the excitation energy, incident laser power and temperature. The intensity of upconverted X_L transition decreases with decreasing laser excitation energy, reflecting the shape of the lower energy flank of the X_L PL line, whereas its dependence on the laser power is sub-linear. We propose that the energy gain required in the UPC of the defect-bound exciton PL originates from an electron Auger recombination between in-gap defect defect states introduced by chalcogen vacancies.

[1] E. Żuberek, M. Majak, J. Lubczyński et al., *Sci Rep* **12**, 13699 (2022).
[2] Y. Zhao, M. Tripathi, K. Čerņevičs et al., *Nat Commun* **14**, 44 (2023).
[3] Y. Zhu, J. Lim, Z. Zhang et al., *ACS Nano* **17** (14), 13545-13553 (2023).