

"Extremely high excitonic g-factors in MoWSe₂ alloy monolayers"

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Monolayers (MLs) of semiconducting transition metal dichalcogenides (S-TMDs), e.g. MoSe₂ and WSe₂, are direct bandgap semiconductors characterized by very interesting optical and electronic properties. S-TMD alloys have emerged as materials with tunable electronic structures and valley polarizations [1].

In this work, we investigate the magneto-optical properties of excitonic complexes in Mo_xW_{1-x}Se₂ MLs encapsulated in hexagonal BN (hBN) with different ratios of Mo and W atoms and compare the results with those achieved for WSe₂ and MoSe₂ MLs. Using low-temperature photoluminescence (PL) experiments carried out in external out-of-plane magnetic fields up to 30 T, we extract the g-factors of the neutral (X) and charged (T) excitons. Under applied magnetic fields, the neutral exciton resonances in S-TMD ML split into two circularly-polarised component due to the Zeeman effect. The energy separation of the σ^\pm components in the B_⊥ field, $\Delta E(B_\perp) = E\sigma^+ - E\sigma^-$ can be expressed as $\Delta E(B_\perp) = g\mu_B B_\perp$ [2], where g denotes the effective g-factor of the neutral exciton and μ_B is the Bohr magneton.

While the measured T g-factors for Mo_xW_(1-x)Se₂ monolayers vary from approximately -3.5 to -5, remaining comparable to those reported for MoSe₂ and WSe₂ monolayers, the g-factors of the X transition exhibit a pronounced composition dependence. Starting from about -4 in MoSe₂, they increase to approximately -4.5 for a Mo concentration of ~85%, -6 for ~70%, -7 for ~50%, and reach values as high as -10 for ~20% Mo content, before returning to about -4 in WSe₂. This striking tunability of the g-factor is verified by first principles calculations of the band structures and angular momenta of MoSe₂ and WSe₂ MLs and their alloys. The calculated values of the g-factors show a trend similar to the experimental ones, and also reveal an additional increase and decrease under application of the compressive or tensile biaxial strains, respectively. Our studies indicate that the alloying of S-TMD MLs is an efficient mechanism to enhance the g-factors of neutral excitons, up to values that have only been observed for interlayer excitons in TMDs heterostructures (HSs) with nearly 0° or 60° twist angles so far [3]. Due to the much simpler fabrication process of MLs compared to TMD HSs with specific twist angles, alloy MLs open new avenues as potential candidates for valleytronic and quantum devices [4].

References

[1] Y. Meng, et al., *Nano Letters* **19** (1), 299-307 (2019).

[2] M. Zinkiewicz, et al., *Nano Letters* **21**, 2519 (2021).

[3] K. L. Seyler, et al., *Nature* **567**, 66 (2019).

[4] S. J. Prado, et al., *Journal of Physics: Condensed Matter* **16**, 6949 (2004).