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

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Monolayers (MLs) of semiconducting transition metal dichalcogenides (S-TMDs), e.g. MoSe<sub>2</sub> and WSe<sub>2</sub>, 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 magneto-optical properties of excitonic complexes in  $Mo_xW_{1-x}Se_2$  MLs encapsulated in hexagonal BN (hBN) with different ratios of Mo and W atoms and compare the results with those achieved for WSe<sub>2</sub> and MoSe<sub>2</sub> MLs. Under applied magnetic fields, the neutral exciton resonances in S-TMD MLs

split into two circularly polarized components as a result of the Zeeman effect. The energy separation of the  $\sigma^{\pm}$  components in the  $B_{\perp}$  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  $\mu_B$  is the Bohr magneton. Using 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 presented in Fig. 1(a).

Although the measured

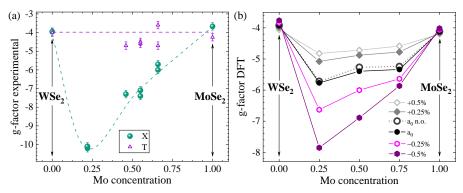


Figure 1: (a) Experimental values of the g-factors extracted for the neutral and charged excitons measured on the MoSe2, WSe2, and MoWSe2 MLs with different Mo/W ratios. (b) Exciton g-factors calculated from the first principles. The colored lines correspond to a(x). The dashed lines indicate the results without optimization of the atomic positions (n.o.), which has a minor impact on the final values.

g-factors for trions in  $Mo_xW_{1-x}Se_2$  MLs vary from around -3.5 to almost -5 and are thus comparable to those of  $MoSe_2$  and  $WSe_2$  MLs, the g-factors for the X transitions change gradually from about -4 for  $MoSe_2$ , to about -6 when the Mo concentration is ~ 70%, to about -7 when it reaches ~ 50%, and even up to about -10 for Mo concentrations of ~ 20%, to then go back to -4 in  $WSe_2$ . This striking tunability of the g-factor is verified by first-principles calculations of the band structures and angular momenta of  $MoSe_2$  and  $WSe_2$  MLs and their alloys. The calculated values of the g-factors (Fig.1 (b)) 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  $0^\circ$  or  $60^\circ$  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).