

Extremely high excitonic g-factors in MoWSe₂ monolayer alloys

K. Olkowska-Pucko¹, T. Woźniak², E. Blundo³, N. Zawadzka¹, Ł. Kipczak¹, J. Szpakowski¹, S. Cianci³, M. Felici³, P. Kapuściński⁴, K. Watanabe⁵, T. Taniguchi⁵, C. Faugeras⁴, M. Potemski⁴, A. Babiński¹, A. Polimeni³, and M. R. Molas¹

¹*Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland*

²*Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland*

³*Physics Department, Sapienza University of Rome, Rome, Italy*

⁴*Laboratoire National des Champs Magnétiques Intenses, CNRS, Grenoble, France*

⁵*National Institute for Materials Science, Tsukuba, Japan*

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 tuneable electronic structures and valley polarizations [1]. Therefore, it is crucial to uncover their basic optical properties.

In this work, we investigate the properties of monolayers (ML) of MoWSe₂ alloys encapsulated in hexagonal boron nitride (hBN) by reflectance contrast (RC) and photoluminescence (PL) experiments performed in external out-of-plane magnetic fields (B_{\perp}) up to 30 T. We examined MLs with different ratio of Mo/W atoms: 0.46/0.54, 0.55/0.45, and 0.66/0.34, as well as the MoSe₂ and WSe₂ MLs.

Under applied magnetic fields, the bright neutral exciton (X) resonances in S-TMD MLs split into two circularly polarised components (σ^{\pm}) due to the Zeeman effect [2]. The σ^{\pm} energy separation can be expressed as $\Delta E(B_{\perp}) = E_{\sigma^+} - E_{\sigma^-} = g\mu_B B_{\perp}$, where g denotes the effective g-factor of the neutral exciton and μ_B is the Bohr magneton. Using this formula, we extracted g-factors values for X transitions for all investigated samples.

As can be seen in the Figure 1, the g-factors of the X transitions extracted for the MoSe₂ and WSe₂ MLs are of the order of -3.7 and -4, respectively. These values are in agreement with the ones reported in the literature [3]. Surprisingly, the corresponding g-factors of the X resonances found in the MLs of the MoWSe₂ alloys exhibit much larger magnitudes. They increase from around the aforementioned -4, through around -6 for the Mo_{0.66}W_{0.34}Se₂ ML, reaching almost -7.5 for the MLs characterized by the about 50/50 ratio of the Mo/W atoms. Moreover, the experimentally obtained values are confirmed by theoretical calculations using density functional theory (DFT), which follow exactly the same trend. The large values of the found g-factors cannot be understood in terms of orbital, valley and spin contributions within few-band models, but come from particular arrangements of bands and their mixing, which can only be captured by DFT calculations.

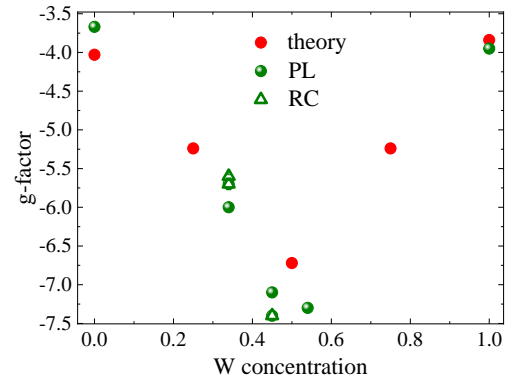


Figure 1. The g-factors for neutral exciton (X) as a function of tungsten (W) concentration in MoWSe₂ MLs. Green and red points correspond to the values of g-factors extracted from experimental data and theoretical calculations, respectively.

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

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

[3] M. Koperski et al., 2D Mater. 6, 015001 (2019).

[4] T. Woźniak et al., Phys. Rev. B 101, 235408 (2021).