Extremely high excitonic g-factors in $MoWSe_2$ monolayer alloys

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Monolayers (MLs) of semiconducting transition metal dichalcogenides (S-TMDs), *e.g.* $MoSe_2$ and WSe_2, 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 $MoWSe_2$ 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 $MoSe_2$ and WSe_2 MLs.

Under applied magnetic fields, the bright neutral exciton (X) resonances in S-TMD MLs split into two circularly polarised components ($\sigma^{\pm}$) due to the Zeeman effect [2]. The $\sigma^{\pm}$ 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.

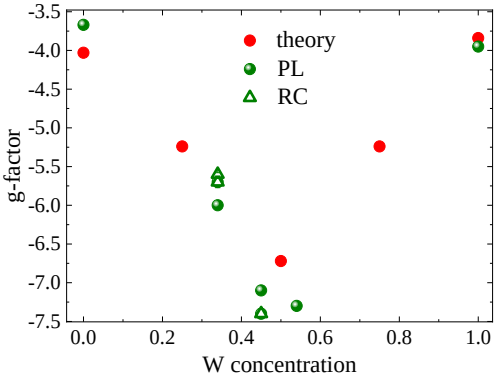

Figure 1. The g-factors for neutral exciton (X) as a function of tungsten (W) concentration in $MoWSe_2$ MLs. Green and red points correspond to the values of g-factors extracted from experimental data and theoretical calculations, respectively.

As can be seen in the Figure 1, the g-factors of the X transitions extracted for the $MoSe_2$ and WSe_2 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 $MoWSe_2$ alloys exhibit much larger magnitudes. They increase from around the aforementioned -4, through around -6 for the $Mo_{0.66}W_{0.34}Se_2$ 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.

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