

Composition-dependent Exciton Engineering in Two-dimensional TMD $\text{Mo}_{1-x}\text{W}_x\text{Se}_2$ Alloys

Muhammad Hussain¹

Omid Ghaebi¹, Mohammad Monfared², Marco Gruenewald¹, Umer Ahsan³, Fedor Lipilin³, Zdenek Sofer³, Ulf Peschel^{2,4}, Giancarlo Soavi^{1,4}

¹Institute of Solid-State Physics, Friedrich Schiller University Jena, Germany.

²Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Germany.

³Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic.

⁴Abbe Center of Photonics, Friedrich Schiller University Jena, Germany.

muhammad.hussain@uni-jena.de

Two-dimensional transition metal dichalcogenide (TMD) alloys provide a versatile platform for broadband tuning of bandgap and excitonic properties through compositional control [1]. Here, we investigate the nonlinear optical response of $\text{Mo}_{1-x}\text{W}_x\text{Se}_2$ alloys, focusing in particular on second harmonic generation (SHG) and two-photon photoluminescence (TP-PL) [2]. We find that varying the W concentration ($x = 0, 0.2, 0.5, 0.75, 1$) enables broadband tuning of the excitonic resonances in the range 1.56 eV to 1.65 eV. In addition, we report that alloyed TMDs exhibit enhanced nonlinearities compared to their pristine counterparts, as illustrated in Fig. 1.

Finally, by combining the resonant energies of SHG and TP-PL and the respective optical selection rules, we are able to extract the energy difference between 1s and 2p exciton states in samples of different alloy composition. By doing this, we find that the exciton binding energy in such alloys varies with W composition (x). This can be used as a parameter to tune not only the optical bandgap, but also the exciton binding energy by changing the alloy composition.

References

1. Tongay, S., et al., *Two-dimensional semiconductor alloys: Monolayer $\text{Mo}_{1-x}\text{W}_x\text{Se}_2$* . Applied Physics Letters, 2014. **104**(1): p. 012101.
2. Hussain, M., et al., *Nonlinear Optical Properties of Mono and Multilayer MoWSe_2 Alloys*. Advanced Optical Materials, 2025. **13**(29): p. e01000.

Figures

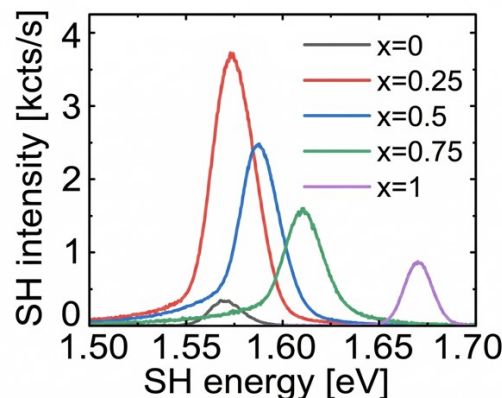


Figure 1: Spectra of composition-dependent SHG at optical resonances.