

## Supplementary Materials

# Filling Exciton Trap-States in Two-Dimensional Tungsten Disulfide ( $WS_2$ ) and Diselenide ( $WSe_2$ ) Monolayers

Zeynep Ezgi Eroglu <sup>1</sup>, Dillon Contreras <sup>1</sup>, Pouya Bahrami <sup>1</sup>, Nurul Azam <sup>2</sup>, Masoud Mahjouri-Samani <sup>2</sup> and Abdelaziz Boulesbaa <sup>1,\*</sup>

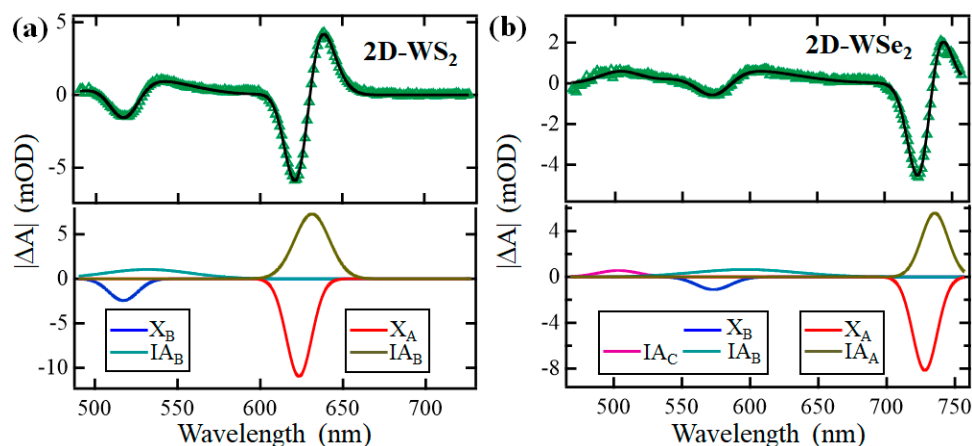
<sup>1</sup> Department of Chemistry & Biochemistry, California State University, Northridge, 18111 Nordhoff Street, Northridge, CA 91330, USA; zeynep.eroglu.568@my.csun.edu (Z.E.E.); dillon.contreras.3@my.csun.edu (D.C.); pouya.bahrami.60@my.csun.edu (P.B.)

<sup>2</sup> Department of Electrical and Computer Engineering, Auburn University, Auburn, AL 36849, USA; mna0018@auburn.edu (N.A.); mzm0185@auburn.edu (M.M.-S.)

\* Correspondence: aboules@csun.edu

### Spectral analysis of transient spectra:

To spectrally resolve the different components of the positive induced absorption (IA) band observed in Figure 2 in the Main Text, we conducted a multi-Gaussian peak fit of transient absorption spectra taken at 10 ps time-delays. This time-delay is chosen because by 10 ps, the IAs resulting from exciton line broadening due to many-body interactions have recovered [1–4]. The returned fitting parameters are listed in Table S1 for 2D- $WS_2$  and Table S2 for 2D- $WSe_2$ .



**Figure S1.** Multi-peak fitting of a transient absorption spectrum collected 10 ps following exciton of the monolayer of 2D- $WS_2$  (a), and 2D- $WSe_2$  (b). The individual components of the fits are shown in the bottom panels.

In the case of 2D- $WS_2$ , we identified four components; two negative peaks corresponding to depletions of excitons  $X_A$  and  $X_B$ , and two positive features  $I_{A_A}$  near  $X_A$  and  $I_{A_B}$  near  $X_B$ . In the case of 2D- $WSe_2$ , an additional  $I_{A_C}$  was identified. We note that the probe used in both samples starts at 480 nm, which allows us to capture the  $I_{A_C}$  in 2D- $WSe_2$ , one expects the existence of a similar IA at shorter wavelengths that we cannot capture using our probe.

**Table S1.** List of the multi-Gaussian peak fit of a transient absorption spectrum measured at 10 ps following excitation of the 2D-WS<sub>2</sub> monolayer at 3.1 eV with 4 J·cm<sup>-2</sup>. I (mOD): peak amplitude; C<sub>0</sub> (nm): peak center; w(nm): full width at half maximum of the peak.

	X <sub>B</sub>	I <sub>A<sub>B</sub></sub>	X <sub>A</sub>	I <sub>A<sub>A</sub></sub>
I (mOD)	-2.45	+1.05	-11.2	+7.4
C <sub>0</sub> (nm)	517.2	531.9	623.4	631.0
w (nm)	20.5	61.4	18.1	24.8

**Table S2.** List of the multi-Gaussian peak fit of a transient absorption spectrum measured at 10 ps following excitation of the 2D-WSe<sub>2</sub> monolayer at 3.1 eV with 2.8 J·cm<sup>-2</sup>. I (mOD): peak amplitude; C<sub>0</sub> (nm): peak center; w(nm): full width at half maximum of the peak.

	I <sub>A<sub>C</sub></sub>	X <sub>B</sub>	I <sub>A<sub>B</sub></sub>	X <sub>A</sub>	I <sub>A<sub>A</sub></sub>
I (mOD)	+0.56	-1.10	+0.65	-8.15	+5.55
C <sub>0</sub> (nm)	503.4	573.1	596.5	728.1	735.2
w (nm)	35.1	29.7	89.3	21.1	22.9

### Supplementary References

1. Sim, S.; Park, J.; Song, J.-G.; In, C.; Lee, Y.-S.; Kim, H.; Choi, H. Exciton dynamics in atomically thin MoS<sub>2</sub>: Interexcitonic interaction and broadening kinetics. *Phys. Rev. B* **2013**, *88*, 075434.
2. Yuan, L.; Huang, L. Exciton dynamics and annihilation in WS<sub>2</sub> 2D semiconductors. *Nanoscale* **2015**, *7*, 7402–7408.
3. Sun, D.; Rao, Y.; Reider, G. A.; Chen, G.; You, Y.; Brezin, L.; Harutyunyan, A. R.; Heinz, T. F. Observation of Rapid Exciton–Exciton Annihilation in Monolayer Molybdenum Disulfide. *Nano Lett.* **2014**, *14*, 5625–5629.
4. Cunningham, P. D.; McCreary, K. M.; Jonker, B. T. Auger Recombination in Chemical Vapor Deposition-Grown Monolayer WS<sub>2</sub>. *J. Phys. Chem. Lett.* **2016**, *7*, 5242–5246.