Supporting Information for:
“Second-harmonic generation enhancement in monolayer transition-metal dichalcogenides by an epsilon-near-zero substrate”

Pilar G. Vianna, Aline dos S. Almeida, Rodrigo M. Gerosa, Dario A. Bahamon, Christiano J. S. de Matos*

MackGraphe – Graphene and Nanomaterials Research Institute, Mackenzie Presbyterian University, São Paulo - 01302-907, Brazil.

* E-mail: cjsdematos@mackenzie.br
1. Second-harmonic generation intensity

To quantify the second-order nonlinear response of a 2D material layer, a monolayer of the material can be considered a nonlinear polarization sheet \( (\chi_s^{(2)}) \) at the interface between two media, in our case, air and the FTO substrate. The second harmonic generation process will depend not only on the nonlinear polarization, but also on the dielectric properties of the surrounding media, which impact the amplitude of the electric field at the interface, as determined by the electromagnetic boundary conditions. With the pump at normal incidence and considering a frequency-dependent refractive indices, the second-harmonic intensity is given by:

\[
I_{SHG}(2\omega) = 2\varepsilon_0 Re\{n_2(2\omega)\} c \left| \frac{4i(2\omega) n_1^2(\omega) \chi_s^{(2)} e \cdot E_1^2(\omega)}{c[n_1(\omega) + n_2(\omega)]^2[n_1(2\omega) + n_2(2\omega)]} \right|^2,  \quad (1)
\]

where \( \omega \) is the pump frequency, \( n_1 \) is the refractive index of the incidence medium, and \( n_2 \) is the substrate refractive index, \( \chi_s^{(2)} \) is the second-order nonlinear sheet susceptibility tensor, \( \hat{e} \) is the unit vector associated to the polarization of the pump field, \( c \) is the speed of light in vacuum and \( \varepsilon_0 \) is the vacuum permittivity. Note that the refractive indices are taken to be complex. As the medium of incidence is air, we make \( n_1(\omega) = n_1(2\omega) = 1 \). In addition, with \( |E_1(\omega)|^2 = \frac{l_1(\omega)}{2 \varepsilon_0 n_1(\omega) c} \), and redefining \( n_2 \) as \( n \) to avoid confusion with the nonlinear refractive index, we get:

\[
I_{SHG}(2\omega) = \frac{8Re\{n(2\omega)\} [2\omega]^2|\chi_s^{(2)} e |^2 l_1^2(\omega)}{\varepsilon_0 c^3 [(1 + n(2\omega))(1 + n(\omega))]^2},  \quad (2)
\]

with \( l_1(\omega) \) being the pump intensity at the incidence, and in which \( |\chi_s^{(2)} e|^2 \) can be replaced with \( |\chi_s^{(2)}|^2 \), with \( \chi_s^{(2)} \) representing the relevant tensor components.

2. Theoretical model

The dielectric function of FTO was described by the Drude free electron model:

\[
\varepsilon = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\gamma \omega},  \quad (3)
\]
where $\varepsilon_{\infty} = 2.95$, $\omega_p = 1.89 \times 10^{15}$ s$^{-1}$ and $\gamma = 0.9 \times 10^{14}$ s$^{-1}$ were obtained by fitting experimental transmission spectra. These fittings are shown in Figures 1(A) and 1(B) for the $p$ polarization at $0^\circ$ and $45^\circ$, respectively, while Figures 2(A) and 2(B) show the fittings for the $s$ polarization at $0^\circ$ and $45^\circ$, respectively.

![Figure S1: Experimental (black) and theoretical (red) transmittance for the $p$ polarization at $0^\circ$ (A) and $45^\circ$ (B).](image1)

![Figure S2: Experimental (black) and theoretical (red) transmittance for the $s$ polarization at $0^\circ$ (A) and $45^\circ$ (B).](image2)

The sample is modeled as a multilayer system with the z-direction normal to the surface. Layer 1 is a semi-infinite vacuum region ($z > 0$) where the pump source is located. Layer 2 corresponds to the FTO substrate of thickness $d$ ($0 > z > -d$), with a monolayer MoS$_2$ sheet on top ($at \ z = 0$) and layer 3 is a semi-infinite glass slide with $z < -d$, where the detector is placed. To evaluate the SHG fields in layer 3, the fundamental fields are first calculated. At normal incidence, the fundamental field at the MoS$_2$ sheet $\vec{E}_\omega = E_\omega \hat{x} = (1 + r_{13}^\omega)E_{i1}\hat{r}$ is related to the incident pump field ($E_{i\omega}^p$) by the Fresnel reflection coefficient:
\[ r_{13}^{\omega} = r_{12} + \frac{t_{12} t_{21} r_{23} \bar{e}^{2k_2d} e^{i2k_2d}}{1 - r_{21} r_{23} e^{i2k_2d}}, \]  

(4)

Note that the coefficients are evaluated at \( \omega \), with

\[ r_{12} = \frac{n_1 - n_2 - Z_0 \sigma^s}{n_1 + n_2 + Z_0 \sigma^s}, \]

and

\[ t_{12} = \frac{2n_1}{n_1 + n_2 + Z_0 \sigma^s}, \]

which accounts for the monolayer MoS\(_2\) contribution through the sheet response

\[ Z_0 \sigma^s = \left( \frac{1}{\varepsilon_0 c} \right) \left[ -(\varepsilon - 1) \varepsilon_0 \omega d \right], \]

where \( d = 0.65 \text{ Å} \), is the effective thickness of the monolayer MoS\(_2\) sheet, \( \varepsilon = 4.97 \) is the dielectric function, \( \varepsilon_0 \) is the vacuum permittivity, and \( n_1, n_2, n_3 \) are the refractive indexes for air, FTO and glass, respectively.

Next, the Green’s function formalism with the infinitesimal vacuum gap approach is used to obtain the SHG fields radiated by the monolayer MoS\(_2\). Using this approach, an infinitesimal vacuum gap is introduced between the MoS\(_2\) layer (at \( z = 0^+ \)) and the FTO layer (at \( 0^- > z > -d \)). The suspended MoS\(_2\) sheet generates a downward (-) and an upward (+) SHG field, defined as:

\[ \vec{E}_\Omega^\pm = i \frac{K_0}{2 \varepsilon_0} (p_{x'}^\Omega \mp \hat{p}_{y'}^\Omega) e^{\pm ik_0 |z|}, \]

(5)

where

\[ K_0 = \frac{\Omega}{c} = 2 \omega \frac{2k_0}{c} = 2k_0, \]

\[ p_{x'}^\Omega = \varepsilon_0 \chi_{s'}^{(2)} \cos (3\theta) \left( \left( 1 + r_{13}^{\omega} \right) E_i^{\omega} \right)^2 \]

and

\[ p_{y'}^\Omega = \varepsilon_0 \chi_{s'}^{(2)} \sin (3\theta) \left( \left( 1 + r_{13}^{\omega} \right) E_i^{\omega} \right)^2. \]

Here, \( \theta \) is the angle between the crystallographic \( x' \) direction (armchair) and the laboratory \( x \) coordinate;

\[ \chi_{s'}^{(2)} = \chi_{s'}^{(2)} y' y' = - \chi_{s'}^{(2)} y y' x = - \chi_{s'}^{(2)} x y x', \]

\[ \chi_{s'}^{(2)} = - \chi_{s'}^{(2)} x y' x'. \]

The second order sheet susceptibility. In this case, we have assumed a time dependence \( e^{-\bar{\alpha} t} \) and defined the \( \hat{s} = \hat{x} \) and \( \hat{p} = \hat{s} \times (\pm K_0) = \mp \hat{y} \) polarization. Both polarizations have been treated separately, \( u = s, p \), and represent the field in the “m\(_h\)” layer by a two-element column vector \( e_{m,u}^u \), where the top (bottom) element described the upward (downward) propagation directions. Therefore, the fields above and below MoS\(_2\) can be written as

\[ e_{1u}^{(0^+)} = v_u + e_{1u}^{(0^-)} = v_u + M_{13}^{u} e_{3u}^{(0^-)} \]

Here, \( v_u \) is an SHG field discontinuity introduced by the monolayer, and \( M_{13}^{u} \) is the transfer matrix. Given that there is no
downward (upward) propagation of the SHG field for \( z > 0^+ \) \((z > d)\), for the s polarization we have:

\[
\left[ \begin{array}{c} E_{1x}^\Omega(0^+) \\ 0 \end{array} \right] = \frac{K_0}{2\epsilon_0} p_{\Omega x}^T \left[ \begin{array}{c} 1 \\ -1 \end{array} \right] + M_{13}^x \left[ \begin{array}{c} 0 \\ E_{3x}^\Omega(-d) \end{array} \right]
\]

(6)

With the transfer matrix defined as:

\[
M_{13}^x = \frac{1}{T_{13}} \left[ \begin{array}{cccc} T_{13} & T_{31} & -R_{13} & R_{31} \\ -R_{31} & T_{13} & 1 & -R_{13} \end{array} \right]
\]

(7)

It is important to highlight that:

i. The transfer matrix \( M_{13}^\mu \) is defined between layer 1 at \( z = 0^- \) and layer 3, so that the transmission \( (T_{ij}) \) and reflection \( (R_{ij}) \) terms do not include the MoS\(_2\) sheet response;

ii. The elements of the transfer matrix are evaluated at \( \Omega = 2\omega \). Using Equation 6 for the s polarization and a similar equation for the p polarization, the field in layer 3, is obtained:

\[
\vec{E}_3^\Omega = \frac{K_0}{2\epsilon_0} (T_{13} p_{\Omega x}^T + T_{13} p_{\Omega y}^T) e^{-iK_0|z|}
\]

(8)

### 2.1 Monolayer MoS\(_2\) on glass

To compare the SHG fields of the MoS\(_2\)/FTO and MoS\(_2\)/glass configurations, the SHG fields for MoS\(_2\) on glass were also calculated. The MoS\(_2\)/glass sample model has two layers, in which layer 1’ is a semi-infinite vacuum layer \((z > 0)\) and layer 2’ \((z < 0)\) is the glass substrate with the monolayer MoS\(_2\) on top. Following the previously detailed methods, we obtain the SHG field in the glass region:

\[
\vec{E}_2^\Omega = \frac{K_0}{2\epsilon_0} (T_{1'2} p_{\Omega x}^{1'2} + T_{1'2} p_{\Omega y}^{1'2}) e^{-iK_0|z|}
\]

(9)
Where, with \( n_1' \) and \( n_2' \) evaluated at \( \Omega = 2\omega \), and \( p_x^\Omega = e_0 x_s^{(2)} \sin (3\theta) \left((1 + r_{12}^{(0)} E_i^{(0)})^2 \right) \) and \( p_y^\Omega = e_0 x_s^{(2)} \sin (3\theta) \left((1 + r_{12}^{(0)}) E_i^{(0)})^2 \right) \). As previously reported, \( r_{12}^{(0)} \) is evaluated at the fundamental frequency and include the MoS\(_2\) sheet response.

### 2.2 Normalized intensity and optical absorption

In order to compare the transmitted field intensity using both substrates, the MoS\(_2\)/FTO SHG intensity (\( I(2\omega)_{FTO} \)) was normalized by the MoS\(_2\)/glass SHG intensity (\( I(2\omega)_{glass} \)), which we define as the enhancement factor (EF):

\[
EF = \frac{I_{123}}{I_{1'2'}} = \frac{I(2\omega)_{FTO}}{I(2\omega)_{glass}} = \frac{|T_{13}(1 + r_{13}^{(0)})^2|^2}{|T_{1'2'}(1 + r_{1'2'}^{(0)})^2|^2} \tag{10}
\]

Given the large wavelength in the FTO substrate around the ENZ condition, the reflection coefficient \( r_{13}^{(0)} \) remains nearly constant as a function of the dielectric thickness of the FTO substrate. Consequently, the EF dependence on the substrate thickness is given by the transmission function \( T_{13} \). Our results remain valid for a broad range of thicknesses as can be observed in Figure 1B (Main text).

It is also important to mention that, as the complex dielectric function of the substrate is used in our model for Fresnel coefficient calculations, absorption is fully accounted for. Figure S3 presents the calculated transmission \( |t_{13}^{(0)}|^2 \), reflection \( |r_{13}^{(0)}|^2 \) and absorption \( A = 1 - |r_{13}^{(0)}|^2 - |t_{13}^{(0)}|^2 \) for the fundamental frequency as function of the thickness. Additionally, the classical skin depth \( \delta = c/\omega \kappa(\omega) \) for FTO is superimposed as the black curve in each panel.

**Figure S3.** (A) Transmission coefficient \( |t_{13}^{(0)}|^2 \). (B) Reflection coefficient \( |r_{13}^{(0)}|^2 \). (C) Absorption \( A = 1 - |r_{13}^{(0)}|^2 - |t_{13}^{(0)}|^2 \). The classical skin depth is represented as the black curve in each panel.
From Figure S3, it is possible to observe that the optical absorption around the ENZ point becomes significant for substrates thicker than 1000 nm. Comparing the optical absorption of the ENZ substrate with the EF map (Figure 1B – Main text), it is evident that an increase in the absorption, reduces the EF. In fact, balance between reflection and moderate absorption around the ENZ point is what defines the observed region with high EF values. For the largest enhancement factor of 9.3 at 1680 nm and a thickness of 520 nm, as in our substrate, we have $|r_{13}|^2 = 0.32$, $A = 1 - |r_{13}|^2 - |t_{13}|^2 = 0.47$ and $\delta = 1046.5$ nm; which is evidence that, despite the substrate absorption around the ENZ point, its thickness is smaller than the classical skin depth and the field is not completely attenuated.

3. FTO substrate characterization and processing

FTO (Fluorine doped tin oxide) deposited on SLG (soda lime glass) commercial samples were kindly provided by MSE Supplies LLC. The original FTO thickness was approximately 600 nm with a sheet resistivity of 7-8 $\Omega/\square$. From AFM topography measurements, Figure S3(A), the films were found to have a root mean square (RMS) roughness of 17.8 nm, which virtually prevented the transfer of monolayer transition metal dichalcogenide (TMD) flakes. Therefore, the FTO substrates were polished with fine-grain diamond sandpaper (1 $\mu$m grit for 3 min, 0.5 $\mu$m grit for 5 min and 0.1 $\mu$m grit for 5 min). The AFM topography after polishing can be observed in Figure S3(B), corresponding to an RMS roughness of approximately 1.7 nm and a measured thickness of 520 nm.

![AFM topography images for the original FTO substrate (A) and for the polished FTO substrate (B).](image)

**Figure S4:** AFM topography images for the original FTO substrate (A) and for the polished FTO substrate (B).
4. MoS\textsubscript{2} and WS\textsubscript{2} Raman and optical microscopy characterization

Raman spectroscopy characterization was performed to confirm the flake thicknesses. Optical microscopy images of the MoS\textsubscript{2} (A) and WS\textsubscript{2} (C) flakes on glass can be observed in Figure S4 and MoS\textsubscript{2} (A) and WS\textsubscript{2} (C) on FTO can be seen in Figure S5.

Figure S4(B) compares spectra from the monolayer and bulk MoS\textsubscript{2} regions of the flake in Figure S4(A), with a wavenumber difference between the A\textsubscript{1g} to E\textsubscript{12g} modes of approximately 18.6 cm\textsuperscript{-1} and 24.5 cm\textsuperscript{-1}, respectively, which is compatible with the literature for monolayer and bulk MoS\textsubscript{2} flakes\textsuperscript{6}. The same features were observed for MoS\textsubscript{2} deposited on FTO, as shown in Figure S5(B).

For the WS\textsubscript{2} flakes, the Raman signature can be observed in Figures S4(D) for the material deposited on the glass substrate and in Figure S5(D) for the 2D material deposited on FTO. It is possible to observe characteristic monolayer feature $I_{2LA(M) + E_{2g}^1}/I_{A_{1g}} > 2$ at the 532-nm wavelength resonant excitation condition, with $I_{2LA(M) + E_{2g}^1}$ being the sum of the intensities in Raman modes $2LA(M)$ and $E_{2g}^1$ and $I_{A_{1g}}$ being the intensity of Raman mode $A_{1g}$\textsuperscript{7}.

**Figure S5:** MoS\textsubscript{2} and WS\textsubscript{2} on glass optical characterization. Optical microscope images of MoS\textsubscript{2} (A) and WS\textsubscript{2} (C) deposited on glass. (B) & (D) Raman spectra obtained at the same color positions marked by a cross in (A) and (C), respectively. Raman data obtained at 532 nm with
0.5 s, 10 accumulations and 3.5 mW laser power for MoS$_2$; and 2 s integration time, 10 accumulations and 1.15 mW laser power for WS$_2$.

Figure S6: MoS$_2$ and WS$_2$ on FTO optical characterization. Optical microscope images of MoS$_2$ (A) and WS$_2$ (C) deposited on FTO. (B) & (D) Raman spectra obtained at the same color positions marked by a cross in (A) and (C), respectively. Raman data obtained at 532 nm with 2 s, 10 accumulations and 3.5mW laser power for MoS$_2$; and 2 s integration time, 10 accumulations and 1.15 mW laser power for WS$_2$.

To minimize possible substrate roughness variations, MoS$_2$ and WS$_2$ flakes were transferred to the same FTO substrate, shown in the optical microscope image of Figure S6. For the samples of TMDs on glass, the glass substrate was the same as the one used for FTO deposition.
5. Sample imaging and flake location

Reflected THG can be observed overlaid on the linear optical image, shown in Figure S8. A red LED source, a CCD camera and some optics were used to optically image, in reflection, both the TMDC flakes and the THG beam profile generated by the pump laser. A neutral density filter is used to control the red LED light intensity (more attenuation on Figure S8(A) and less attenuation on Figure S8(B)), which allows for a better visualization of the THG spot. Also, adjusting the CCD camera’s RGB response improves visualization. THG arises from both FTO and the 2D material (with the spot getting brighter on flakes), which is not a problem, since it is simply used for visualization. The yellow triangle in Figure S8(A) delimits the monolayer flake, which can be more easily seen in Figure S8(B).

Figure S8. Optical image of the flakes under red LED light illumination and the THG beam. (A) Attenuated red LED light. The yellow triangle delimits the monolayer TMDC flake. (B) Higher LED light intensity on the sample.
6. SHG polarization dependence in FTO

As the FTO is deposited by sputtering, it tends to be amorphous, with the observed SHG component possibly arising from some local remnant (and variable) crystallinity. As a consequence, the SHG polarization dependence (parallel configuration) is variable (remaining inexistent in the perpendicular configuration), as shown in Figure S9, for multiple positions of the same substrate. For that reason, as mentioned in the manuscript, the analysis mainly focuses on the perpendicular polarization configuration, considered interference-free from the FTO SHG.

Figure S9. SHG intensity as a function of pump polarization angle in the parallel polarization configuration for FTO at different positions of the same substrate.

7. Theoretical curves for the SHG polarization dependence in the perpendicular configuration
For MoS$_2$ in the perpendicular configuration, the theoretical prediction is shown below, in Fig. S10. The red plot represents the SHG intensity as a function of the pump polarization angle for MoS$_2$/FTO and the black plot for MoS$_2$/Glass. Data has been shifted by 9° and 6° in the FTO and Glass plots, respectively, to reflect the experimental crystal orientations.

![Figure S10. Theoretical prediction for MoS$_2$ on FTO (red) and Glass (black) in the perpendicular polarization.](image)

For WS$_2$, theoretically predicting the SHG polarization dependence would only be meaningful in a strain-controlled experiment. Without the nature (uniaxial, biaxial), direction, and local strain amplitude, such calculation would be difficult and of limited applicability. For simplicity, we could assume the monolayer WS$_2$ is under uniaxial strain$^{10,11}$, however, a number of free-parameters would have to be implied, and no consistent model or useful data extracted, as more sophisticated methods would be necessary to model the nature of the strain in our samples.

8. SHG polarization dependence for TMDCs on Glass

MoS$_2$/Glass and WS$_2$/Glass in the parallel configuration present the same pattern and intensity as in the perpendicular configuration with a phase shift of of 30°, as shown in the Fig. S11. The results for MoS$_2$/Glass can be observed in Fig. S11 (A) and WS$_2$/Glass in Fig. S11 (B).
9. Photoluminescence measurements

During sample preparation, TMDC flakes were exfoliated on PDMS, which in contact with the desired substrates and then detached, transferred the monolayers to glass and FTO. The procedure relies on pressure applied during the transfer process, which can possibly deform the viscoelastic stamp, yielding strain. The origin of strain is usually attributed to the inherent lack of stiffness of PDMS. PDMS being soft can get slightly deformed during transfer by the pressure exerted upon contact with the target substrate, likely being the deformation source to induce strain in the flake being transferred.

In principle, and as already observed by others, the photoluminescence (PL) shift can be considered an indicator of how the electronic band structure is altered by the application of strain in TMDCs. In our case, PL for monolayer WS$_2$ was measured before and after the transfer process. Figure S12 shows the normalized PL for monolayer WS$_2$ on PDMS and after transferring to FTO (A) and Glass (B). It is possible to observe a shift in the PL peaks, both from 2.02 eV to 2.01 eV, compatible with tensile strain of less than 1% in monolayer WS$_2$. This strain magnitude is compatible with the observed deformation in the SHG polarization dependent plots in Fig. 4(B).
Figure S12. Normalized PL for WS$_2$ monolayers on PDMS (red curve) and after transferring to FTO (A) and Glass (B).

References:

(1) Shen, Y. R. OPTICAL SECOND HARMONIC GENERATION AT INTERFACES. *Annu. Rev. Phys. Chem.* 1989, 40, 327–350.
(2) Li, Y.; Heinz, T. F. Two-Dimensional Models for the Optical Response of Thin Films. *2D Mater.* 2018, 5 (2).
(3) Sipe, J. E. New Green-Function Formalism for Surface Optics. *J. Opt. Soc. Am. B* 1987, 4 (4), 481.
(4) Sipe, J. E.; Moss, D. J. Phenomenological Theory of Optical Second- and Third-Harmonic Generation from Cubic Centrosymmetric Crystals. *Phys. Rev. B* 1987, 35 (3), 1129–1141.
(5) Dean, J. J.; Van Driel, H. M. Graphene and Few-Layer Graphite Probed by Second-Harmonic Generation: Theory and Experiment. *Phys. Rev. B - Condens. Matter Mater. Phys.* 2010, 82 (12), 1–10.
(6) Lee, C.; Yan, H.; Brus, L. E.; Heinz, T. F.; Hone, J.; Ryu, S. Anomalous Lattice Vibrations of Single- and Few-Layer MoS2. *ACS Nano* 2010, 4 (5), 2695–2700.
(7) Berkdemir, A.; Gutiérrez, H. R.; Botello-Méndez, A. R.; Perea-López, N.; Elías, A. L.; Chia, C. I.; Wang, B.; Crespi, V. H.; López-Urias, F.; Charlier, J. C.; et al. Identification of Individual and Few Layers of WS2 Using Raman Spectroscopy. *Sci. Rep.* 2013, 3, 1–8.
(8) Wang, Z.; Chen, C.; Wu, K.; Chong, H.; Ye, H. Transparent Conductive Oxides and Their Applications in Near Infrared Plasmonics. *Phys. Status Solidi Appl. Mater. Sci.* 2019, 216 (5), 1–12.
(9) Koirala, M. P.; Joshi, L. P. Structural and Optical Properties of Fluorine Doped Tin Oxide Thin Film Deposited by Home Built Spray Pyrolysis Unit. *Himal. Phys.* 2017, 6, 58–60.
(10) Liang, J.; Zhang, J.; Li, Z.; Hong, H.; Wang, J.; Zhang, Z.; Zhou, X.; Qiao, R.; Xu, J.; Gao, P.; et al. Monitoring Local Strain Vector in Atomic-Layered MoSe2 by Second-Harmonic Generation. *Nano Lett.* 2017, 17 (12), 7539–7543.
(11) Mennel, L.; Furchi, M. M.; Wachtler, S.; Paur, M.; Polyushkin, D. K.; Mueller, T. Optical Imaging of Strain in Two-Dimensional Crystals. *Nat. Commun.* 2018, 9 (516).
(12) Castellanos-Gomez, A.; Buscema, M.; Molenaar, R.; Singh, V.; Janssen, L.; van der Zant, H. S. J.; Steele, G. A. Deterministic Transfer of Two-Dimensional Materials by All-Dry Viscoelastic Stamping. *2D Mater.* 2014, 1, 011002.
(13) Jain, A.; Bharadwaj, P.; Heeg, S.; Parzefall, M.; Taniguchi, T.; Watanabe, K.; Novotny, L. Minimizing Residues and Strain in 2D Materials Transferred from PDMS.
(14) Pak, S.; Lee, J.; Lee, Y. W.; Jang, A. R.; Ahn, S.; Ma, K. Y.; Cho, Y.; Hong, J.; Lee, S.; Jeong, H. Y.; et al. Strain-Mediated Interlayer Coupling Effects on the Excitonic Behaviors in an Epitaxially Grown MoS2/WS2 van Der Waals Heterobilayer. *Nano Lett.* 2017, 17 (9), 5634–5640.

(15) Aas, S.; Bulutay, C. Strain Dependence of Photoluminescence and Circular Dichroism in Transition Metal Dichalcogenides: A k · p Analysis. *Opt. Express* 2018, 26 (22), 28672.

(16) Tyrnina, A. V.; Bandurin, D. A.; Khestanova, E.; Kravets, V. G.; Koperski, M.; Guinea, F.; Grigorenko, A. N.; Geim, A. K.; Grigorieva, I. V. Strained Bubbles in van Der Waals Heterostructures as Local Emitter of Photoluminescence with Adjustable Wavelength. *ACS Photonics* 2019, 6.

(17) Manzeli, S.; Allain, A.; Ghadimi, A.; Kis, A. Piezoresistivity and Strain-Induced Band Gap Tuning in Atomically Thin MoS2. *Nano Lett.* 2015, 15 (8), 5330–5335.