*Contribution (Oral)*

# Bandgap tuning of single-layer transition metal dichalcogenides under biaxial strain

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Strain engineering has been proposed as a promising route to modify the electronic and optical properties of two-dimensional (2D) materials [1]. These materials can stand to large mechanical deformations, of the order of 10%, while conventional 3D semiconductors tend to break at moderate deformations of 0.5-1.5%. Another key feature of strain engineering of 2D materials stands in the way in which they can be strained. In fact, while 3D systems are typically stressed by epitaxial growing them onto substrates with a certain lattice parameter mismatch, strain in 2D systems can be applied by stretching [2] or bending [3]. Experiments on $MoS_2$ single-layer and few-layers flakes have already demonstrated that the optical band gap can be changed of 50 meV/% for uniaxial strain and of 100 meV/% for biaxial strain. Most of these strain engineering experiments to date, however, study uniaxial tensile strain under static conditions and, apart from few exceptions, are limited to $MoS_2$. In this talk I will present results on biaxial straining, both tensile and compressive, of single-layer transition metal dichalcogenides (TMDC). We studied the effect of strain on mechanically exfoliated flakes of monolayer $MoS_2$ deposited on different polymeric substrates. We apply the strain exploiting the large mismatch between the thermal expansion coefficients of the polymeric substrates and the fabricated TMDCs flake deposited on top. We studied the substrate dependency of the strain transfer efficiency and we find that for substrates with Young's modulus larger than 1 GPa, biaxial strain can be applied reproducibly without slippage. We investigate the effects of strain on the optical properties of single-layers $MoS_2$, $MoSe_2$, $WS_2$ and $WSe_2$ and we observe a redshift of the optical band gap of these 2D TMDCs for increasing tensile strain. The observed bandgap shifts as a function of substrate extension/compression follow the order $MoSe_2 < MoS_2 < WSe_2 < WS_2$, i.e. with $WS_2$ providing the largest bandgap tunability and $MoSe_2$ the lowest. This method can be readily applied to other 2D materials and be used to vary the strain in real time.

## References

[1] Roldan, R., et al., Strain engineering in semiconducting two-dimensional crystals. *J. Phys. Condens. Matter.* **27**, (2015) 313201.

[2] He, K., et al., Experimental demonstration of continuous electronic structure tuning via strain in atomically thin $MoS_2$. *Nano Lett.* **13**, (2013) 2931-6.

[3] Lloyd, D., et al., Band Gap Engineering with Ultralarge Biaxial Strains in Suspended Monolayer $MoS_2$. *Nano Lett.* **16**, (2016) 5836-41.