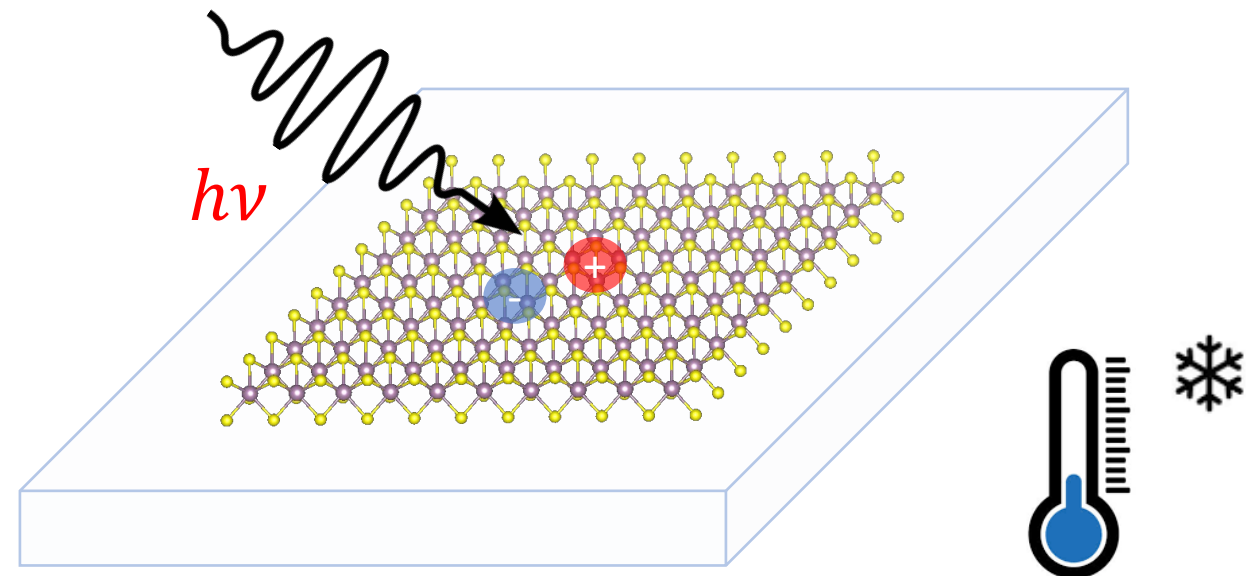




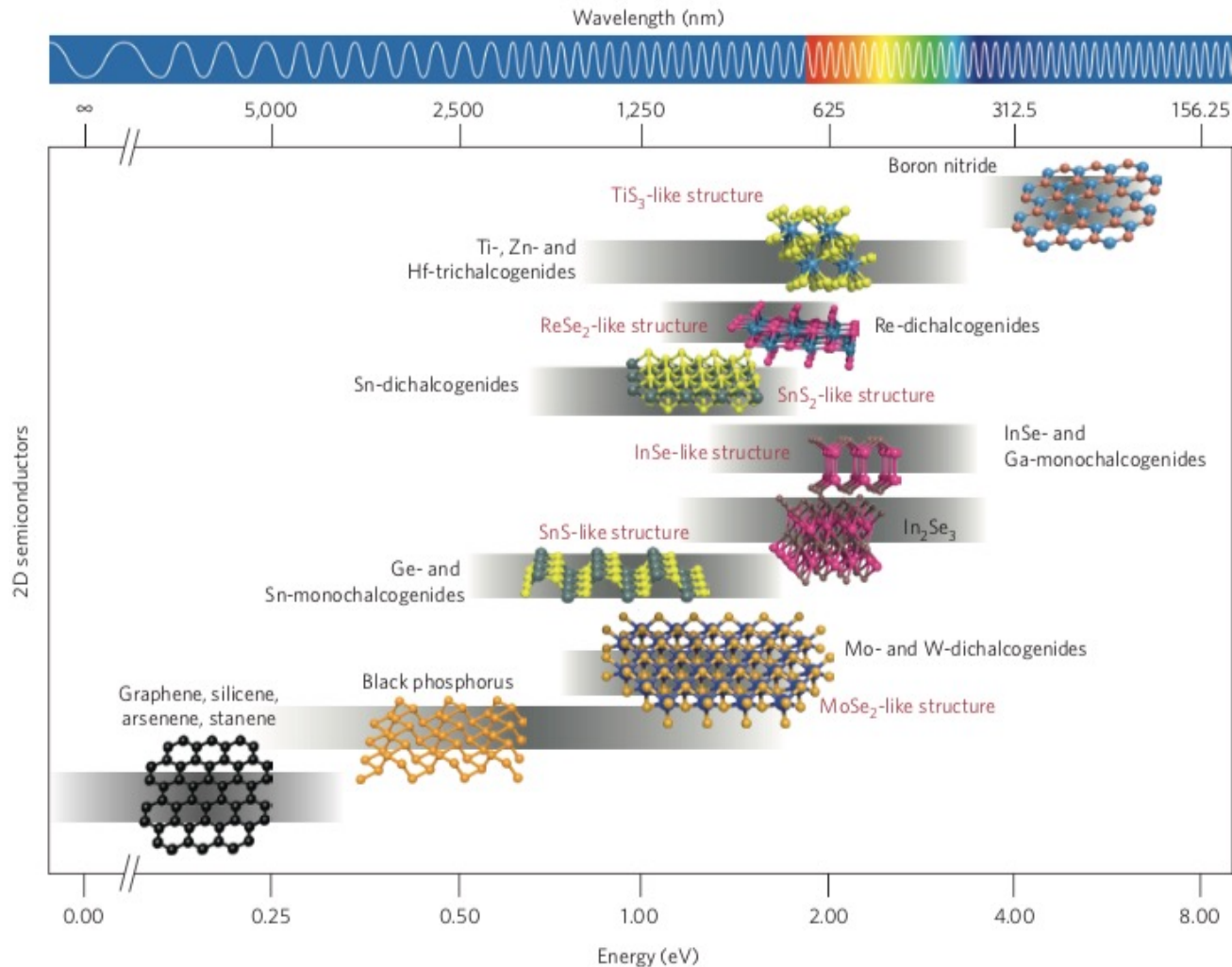
# Biaxial compressive strain tuning of neutral and charged excitons in single-layer transition metal dichalcogenides

Reyes Calvo

*Departamento de Física Aplicada (DFA)*  
*Instituto Universitario de Materiales (IUMA)*  
*Universidad de Alicante*



# 2D semiconductors



➤ Emergent properties at the 2D limit

➤ Excitonic states

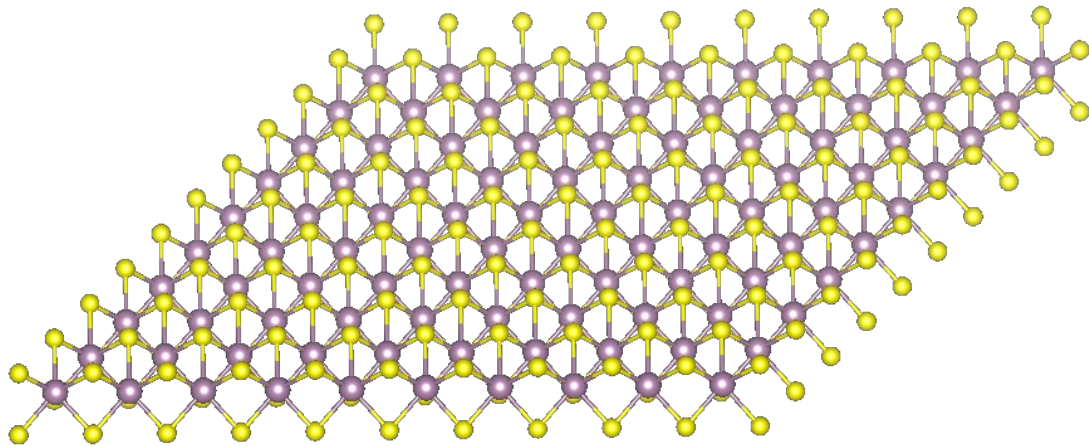
➤ Tunability

➤ Strain engineering

# 2D semiconductors

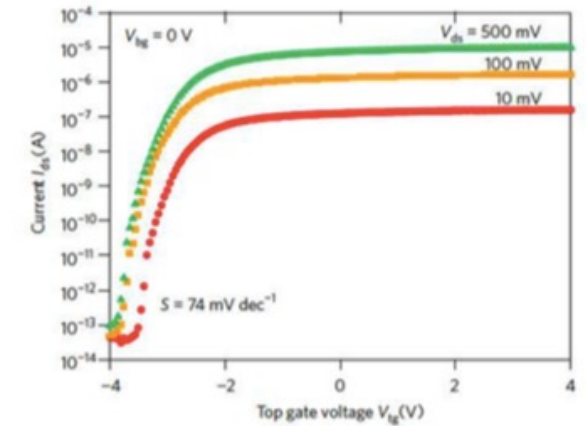
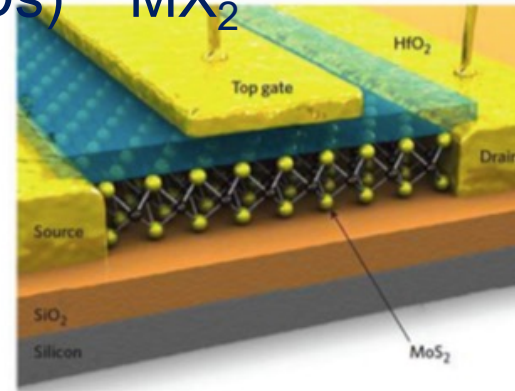
MoS<sub>2</sub>

Transition Metal Dichalcogenides (TMDs) MX<sub>2</sub>

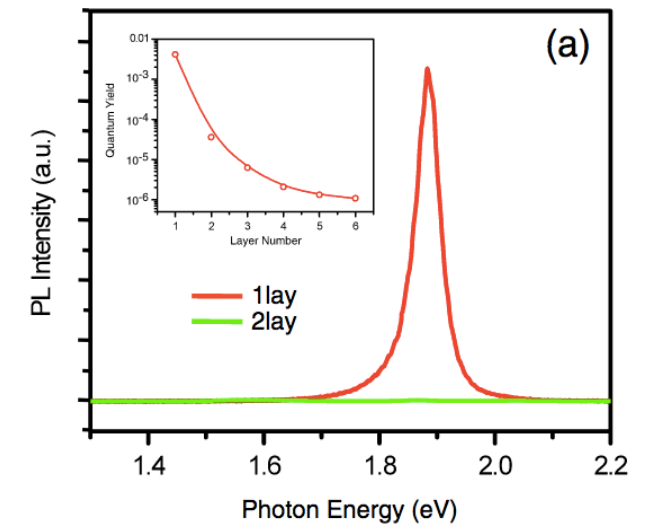
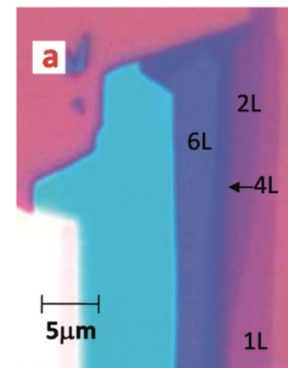


M: Mo, W

X: S, Se, Te

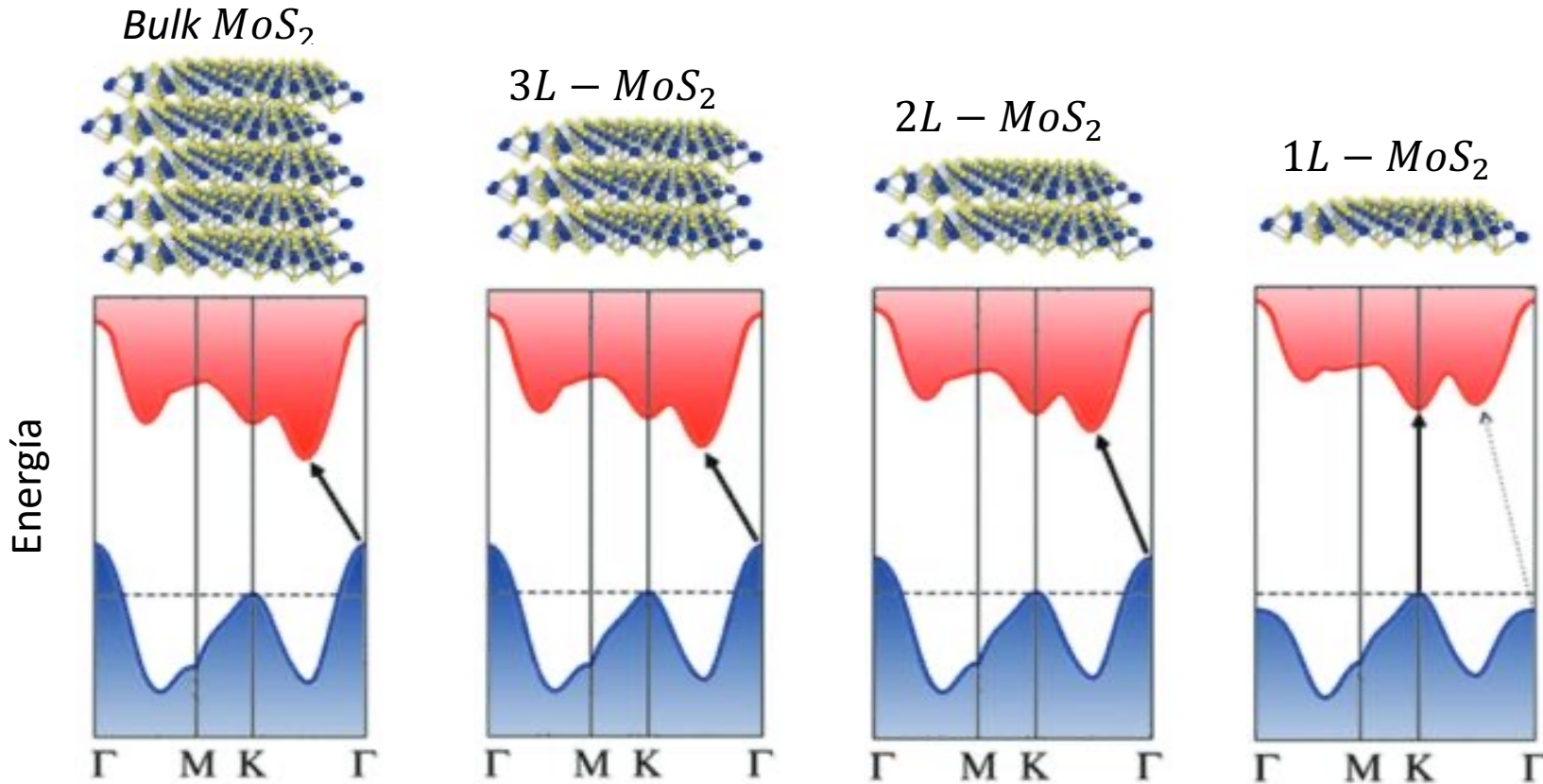


B. Radisavljevic et al., Nature Nano. 6, 147 (2011)



Mak et al. Phys. Rev. Lett. 105, 136805 (2010)

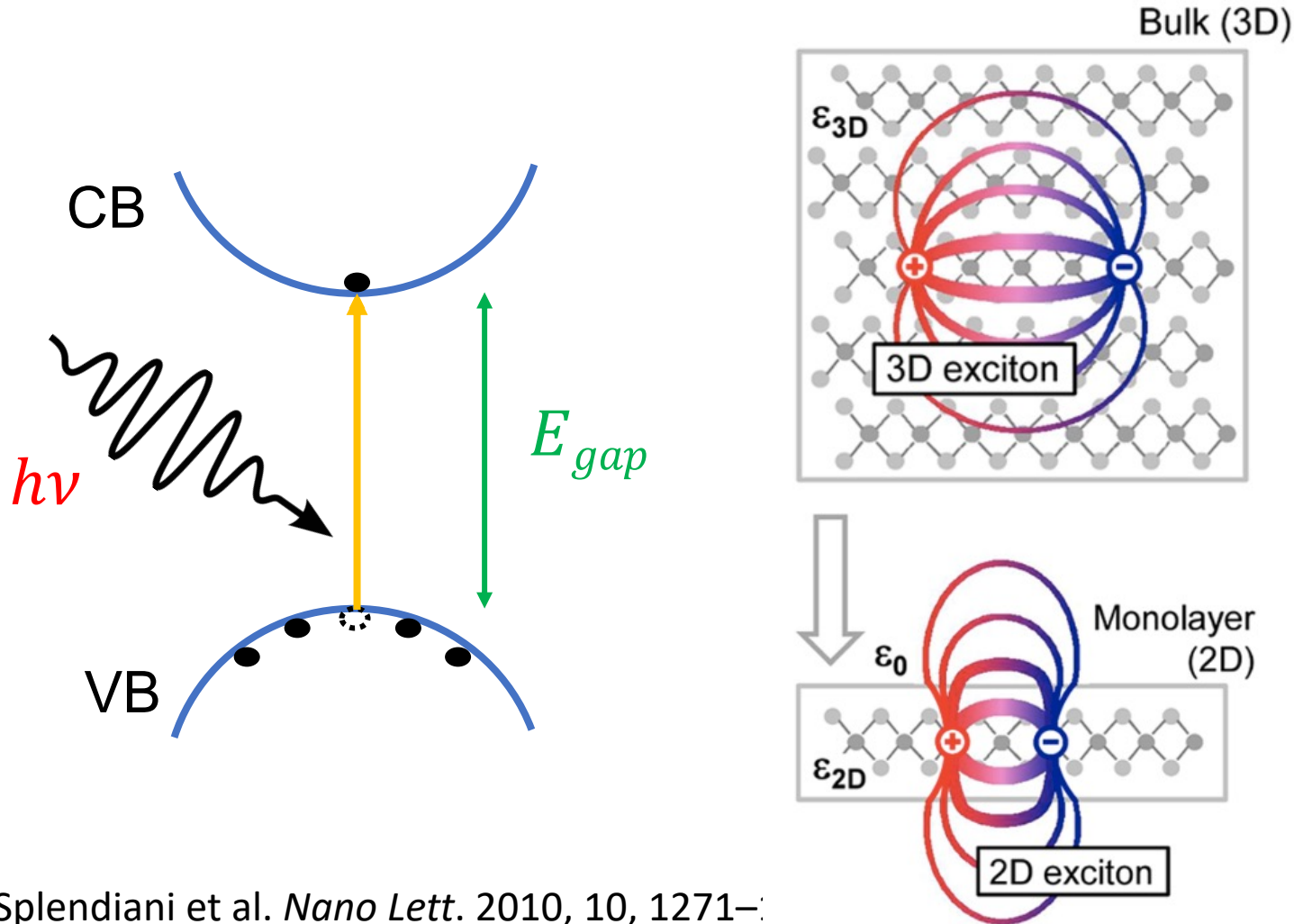
# Single-layer TMDs: excitonic properties



At the single layer limit:

➤ Direct Bandgap

# Single-layer TMDs: excitonic properties



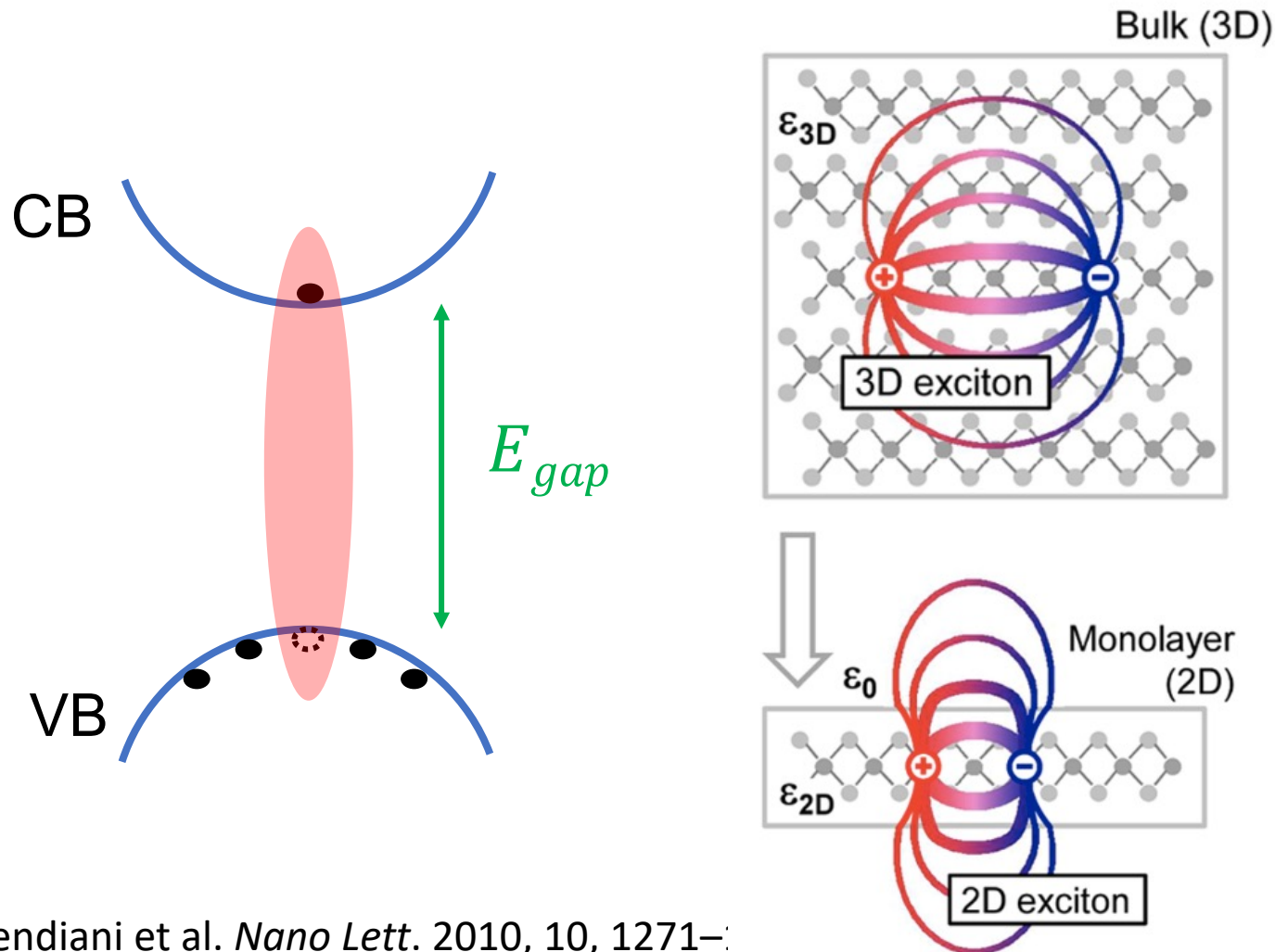
Splendiani et al. *Nano Lett.* 2010, 10, 1271–

Chernikov et al. *PRL* 113, 076802 (2014)

At the single layer limit:

- Direct Bandgap
- Reduced dielectric screening

# Single-layer TMDs: excitonic properties



Splendiani et al. *Nano Lett.* 2010, 10, 1271–  
Chernikov et al. *PRL* 113, 076802 (2014)

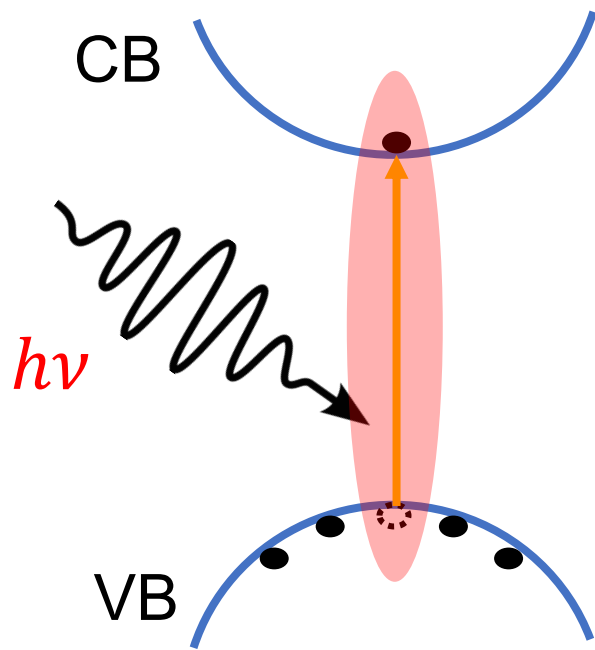
At the single layer limit:

- Direct Bandgap
- Reduced dielectric screening
- Bound states: **excitons**

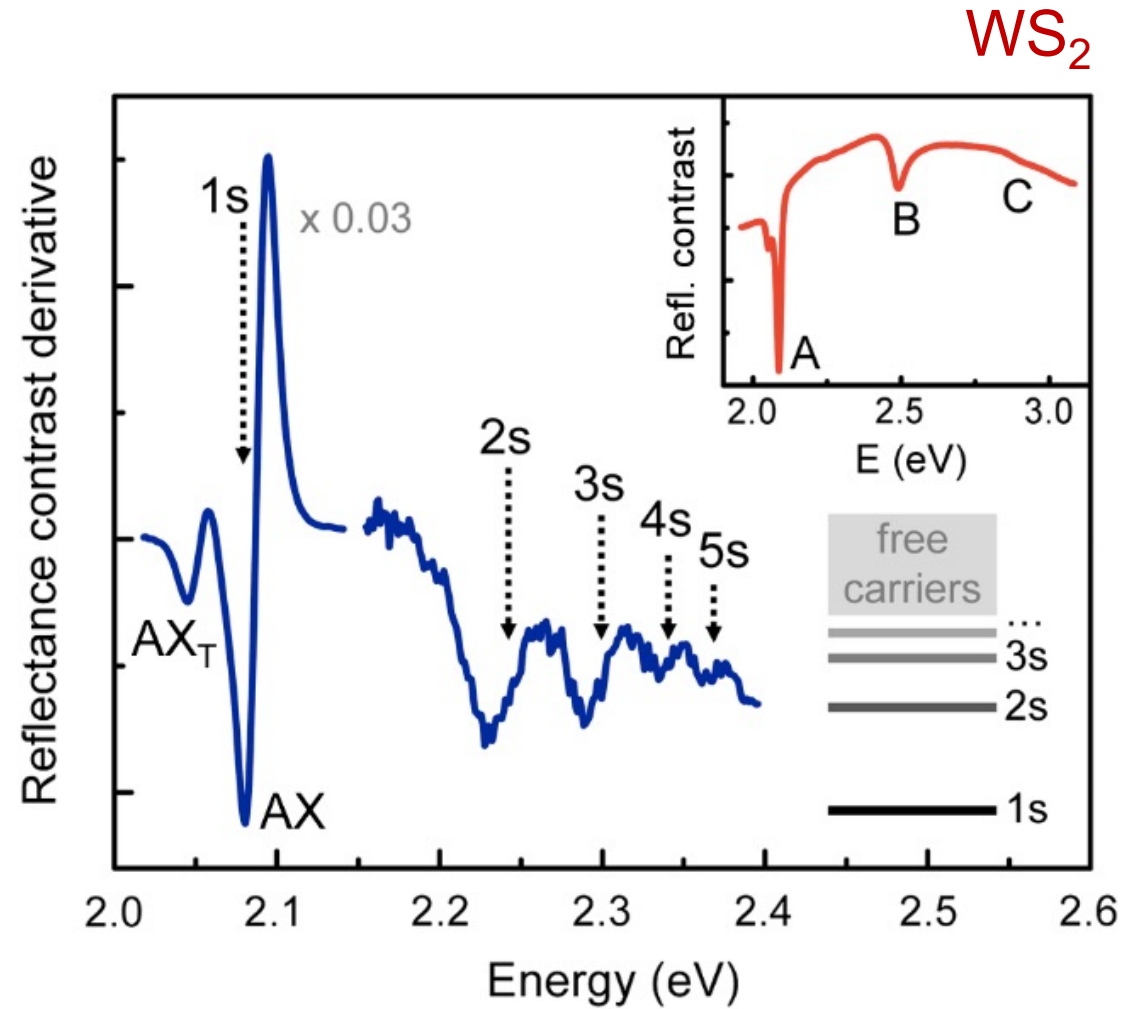
$$E_{\text{exciton}} = E_{\text{gap}} - E_{\text{binding}}$$

$$E_{\text{binding}} (\text{MoS}_2) \sim 500 \text{ meV} \gg k_B T$$

# Single-layer TMDs: excitonic properties



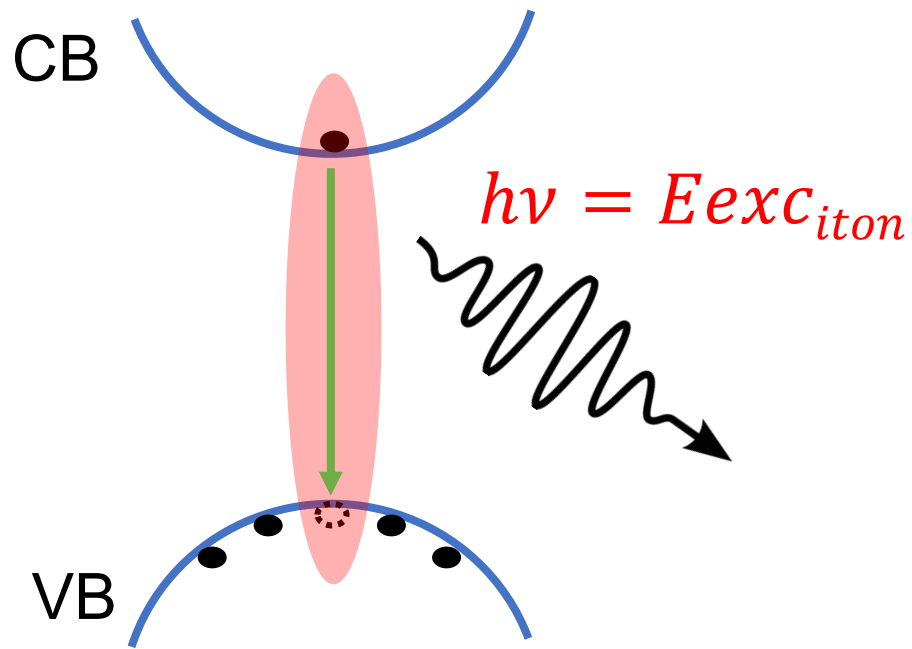
Absorption



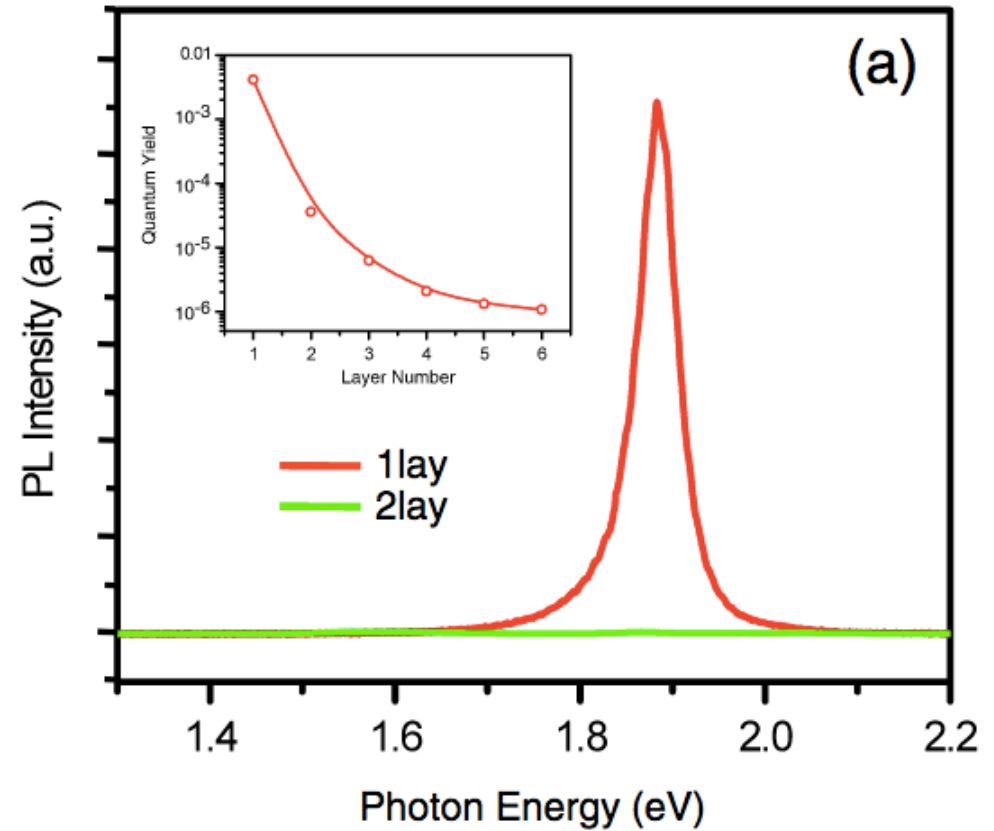
Chernikov et al. *PRL* 113, 076802 (2014)

# Single-layer TMDs: excitonic properties

MoS<sub>2</sub>



Photoluminescence

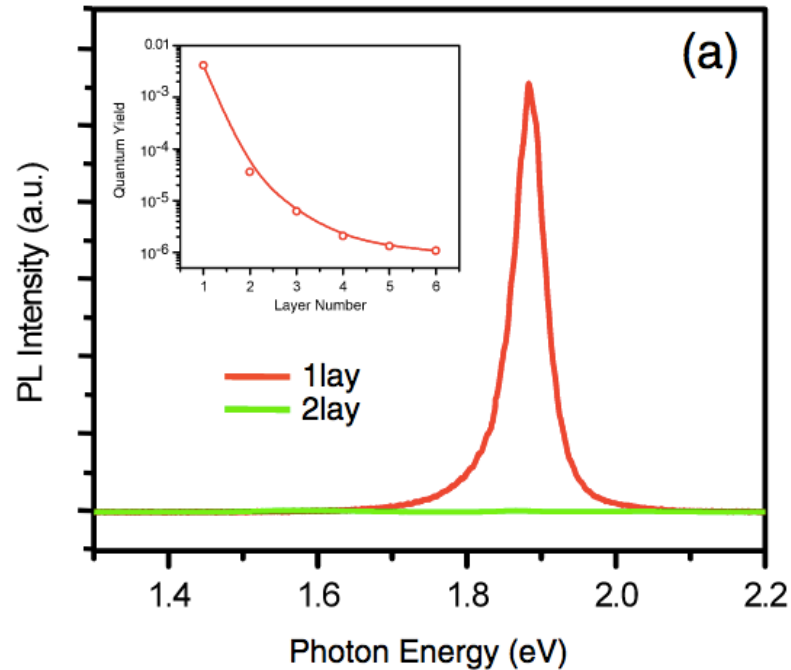


Mak et al. Phys. Rev. Lett. 105, 136805 (2010)

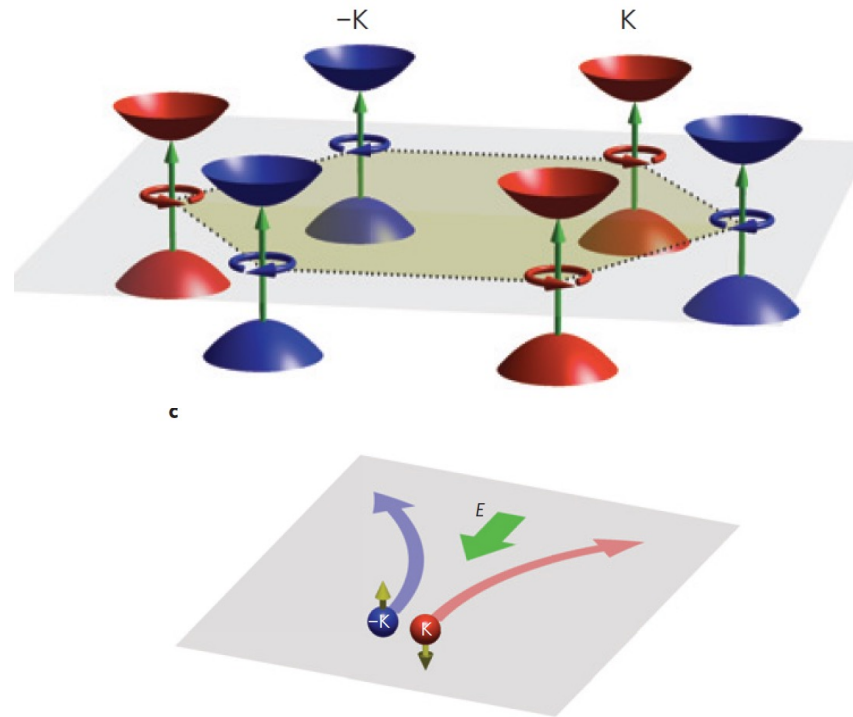


# Single-layer TMDs: excitonic properties

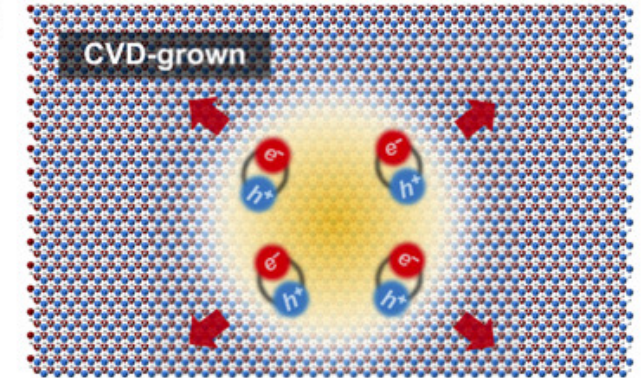
Light emission devices



Valleytronics/Spintronics



Exciton Transport devices

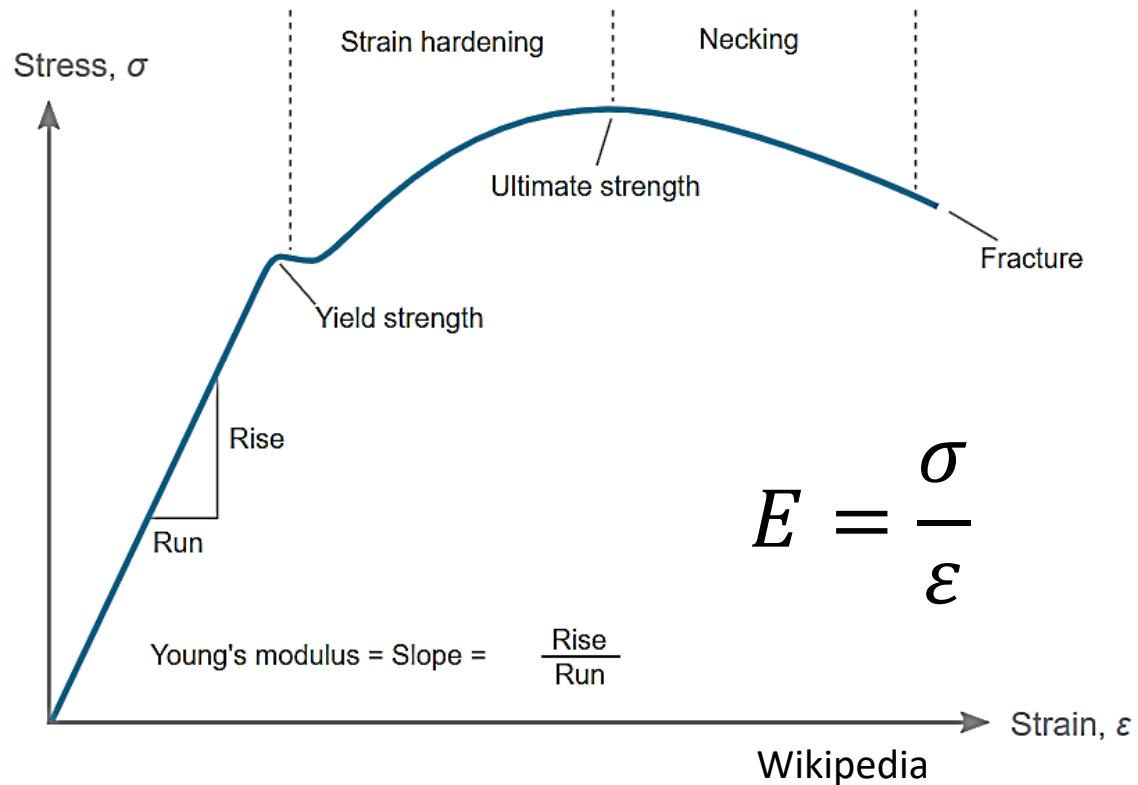


Liue et al. Adv.Mater.2020, 32, 1906540

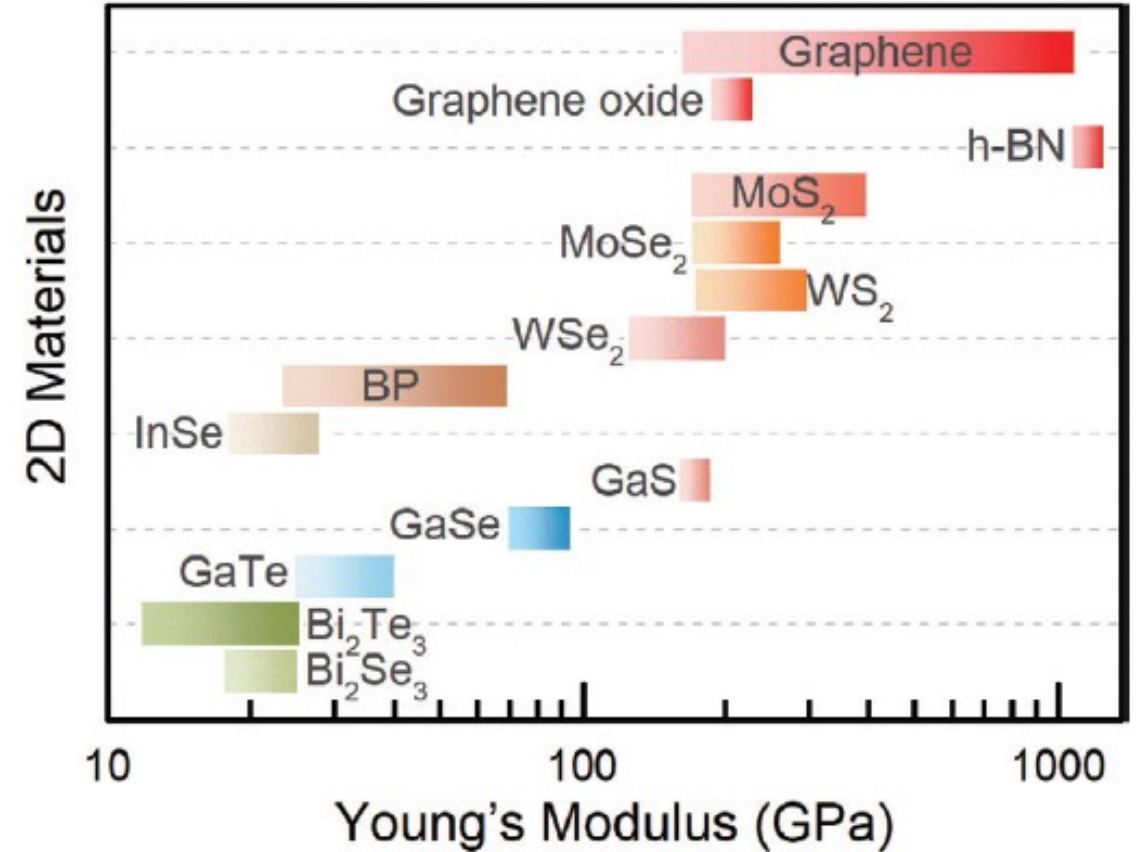
Mak et al. Phys. Rev. Lett. 105, 136805 (2010)

Xu et al. Nature Physics 10, 343–350 (2014)

# Strain engineering in 2D materials



Du, J (2021). Small Methods, 5(1), 2000919.v



$$K = E \times \frac{A}{L}$$

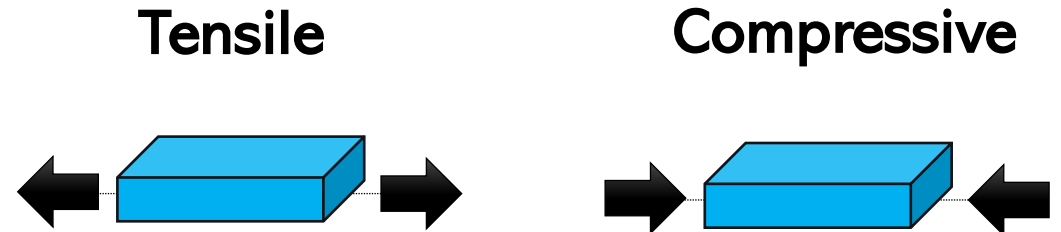
➤ Single-layer TMDs exhibit a remarkable resilience to mechanical deformation.

# Strain engineering in 2D materials

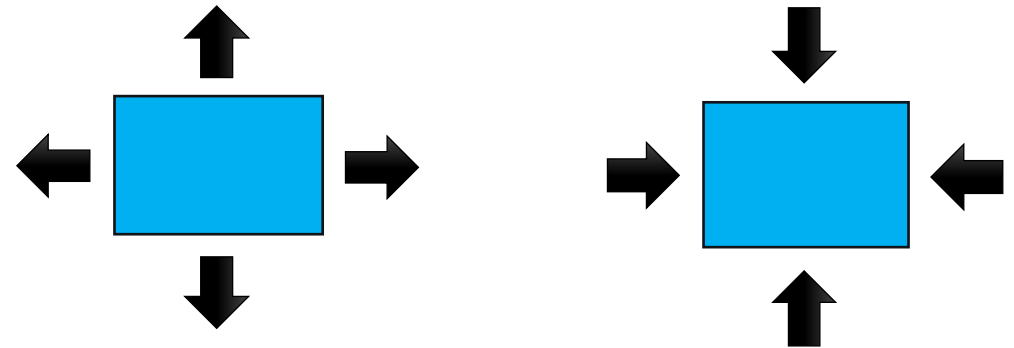
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Depending on degrees of freedom

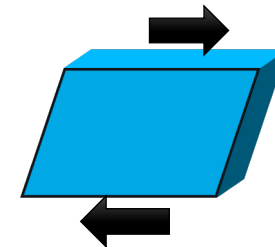
☐ Uniaxial



☐ Biaxial



☐ Shear

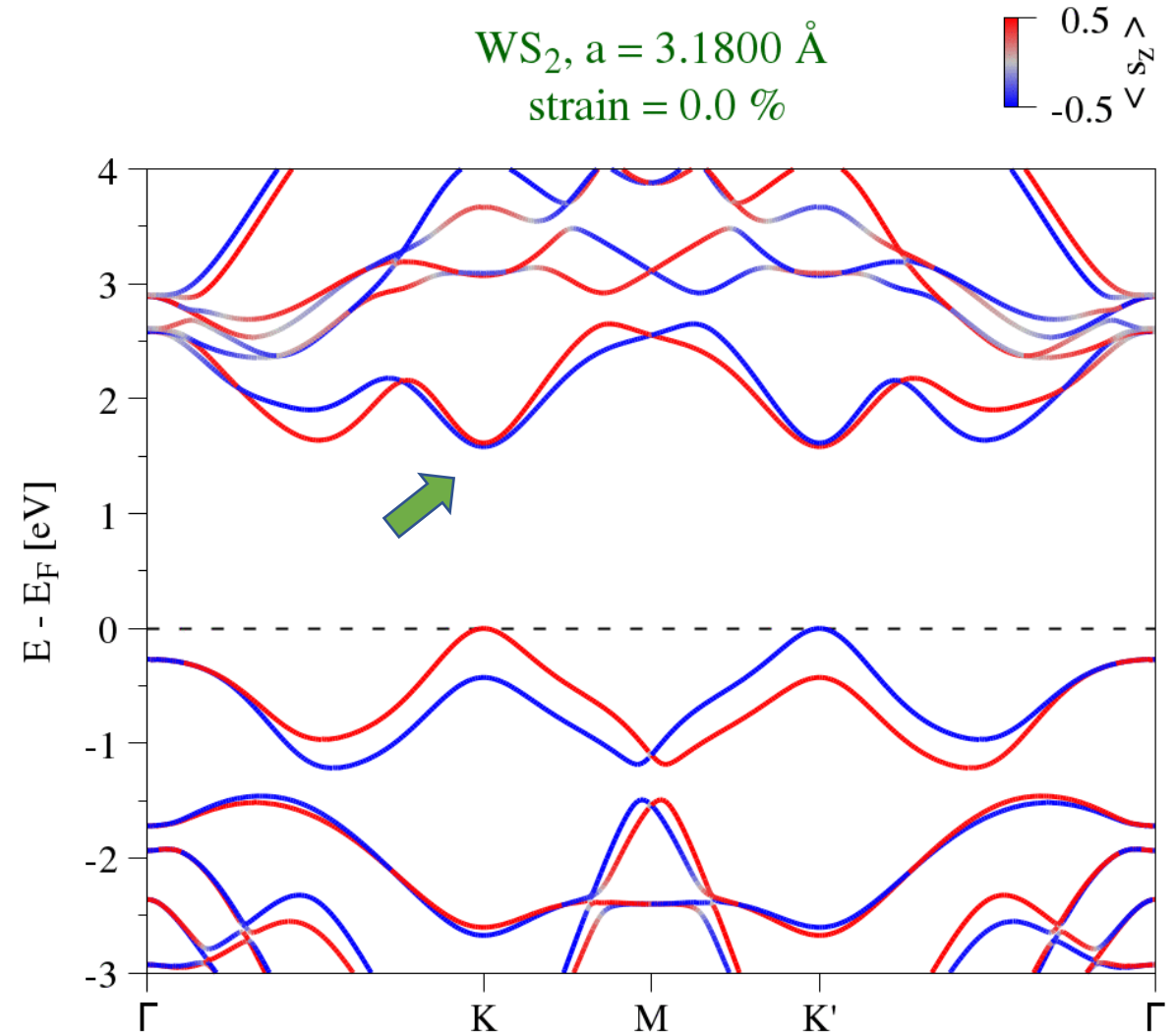
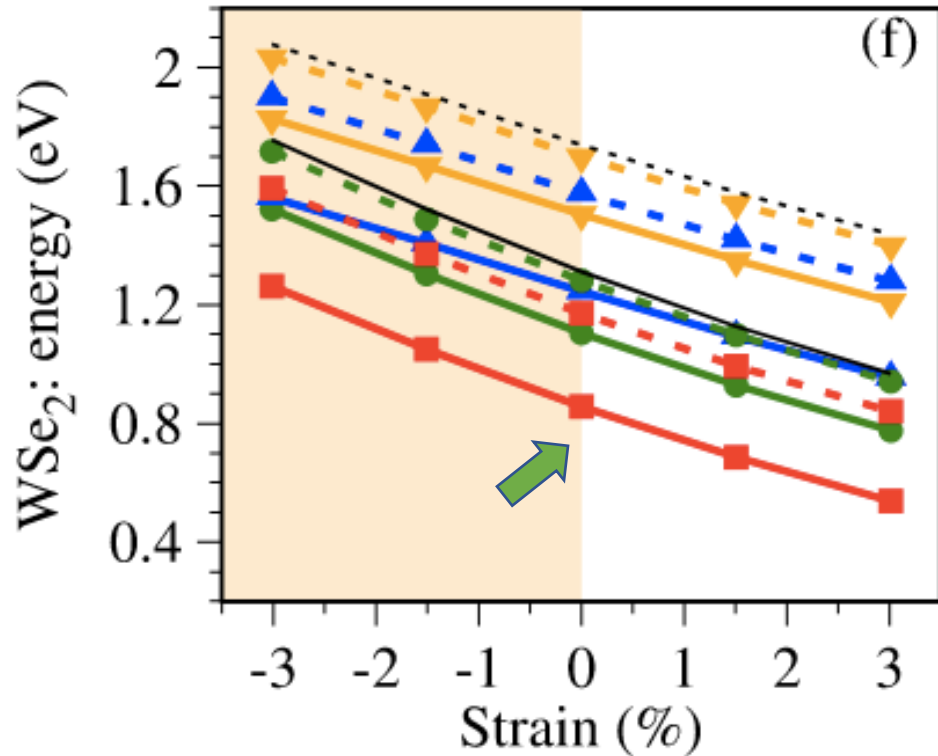
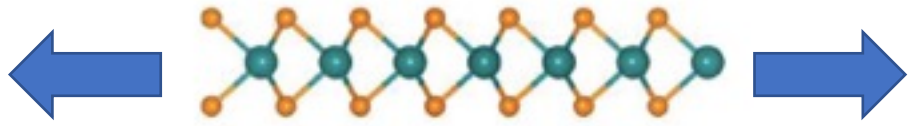


$$S = \frac{L - L_0}{L_0} 100\%$$

# Strain engineering in 2D materials

Zollner, K., Junior, P. E. F., & Fabian, J. (2019). Physical Review B, 100(19), 195126.

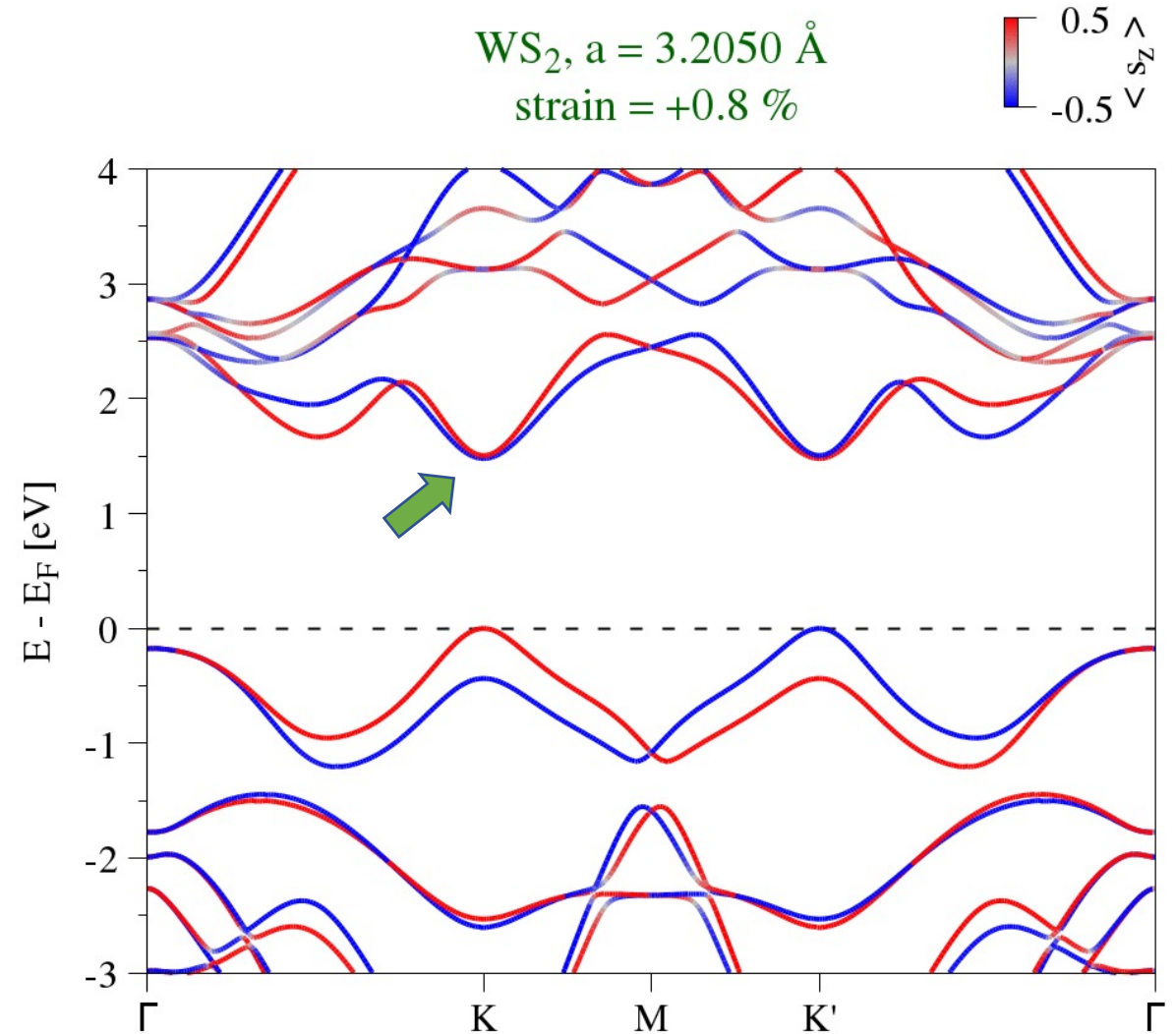
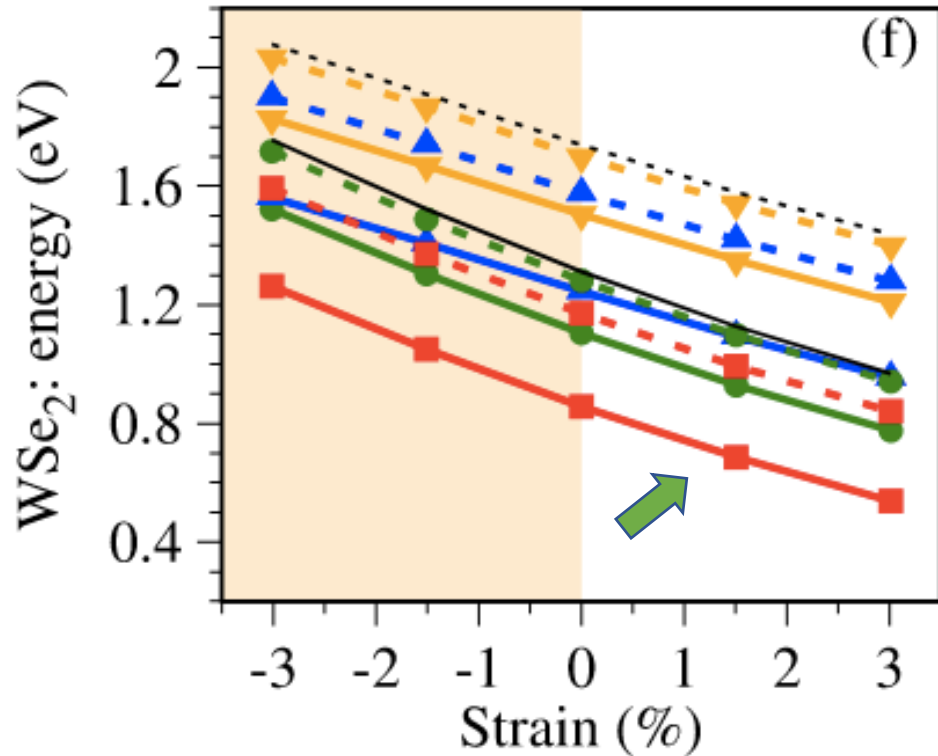
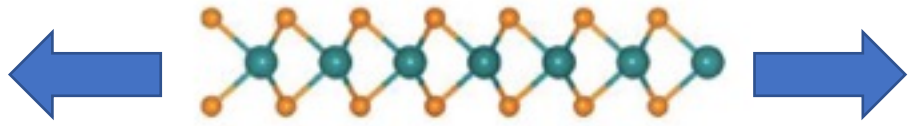
## Tensile strain



# Strain engineering in 2D materials

Zollner, K., Junior, P. E. F., & Fabian, J. (2019). Physical Review B, 100(19), 195126.

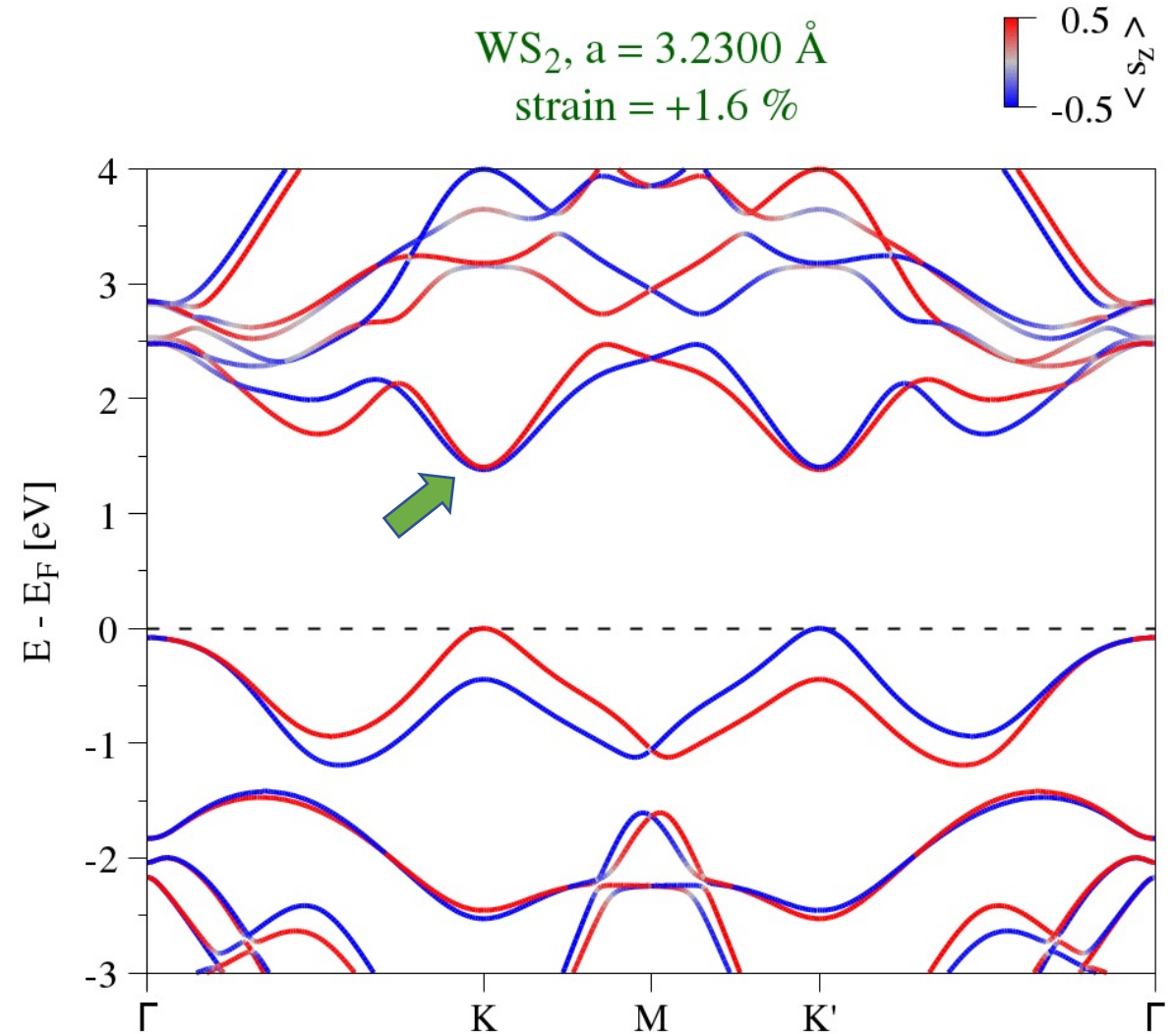
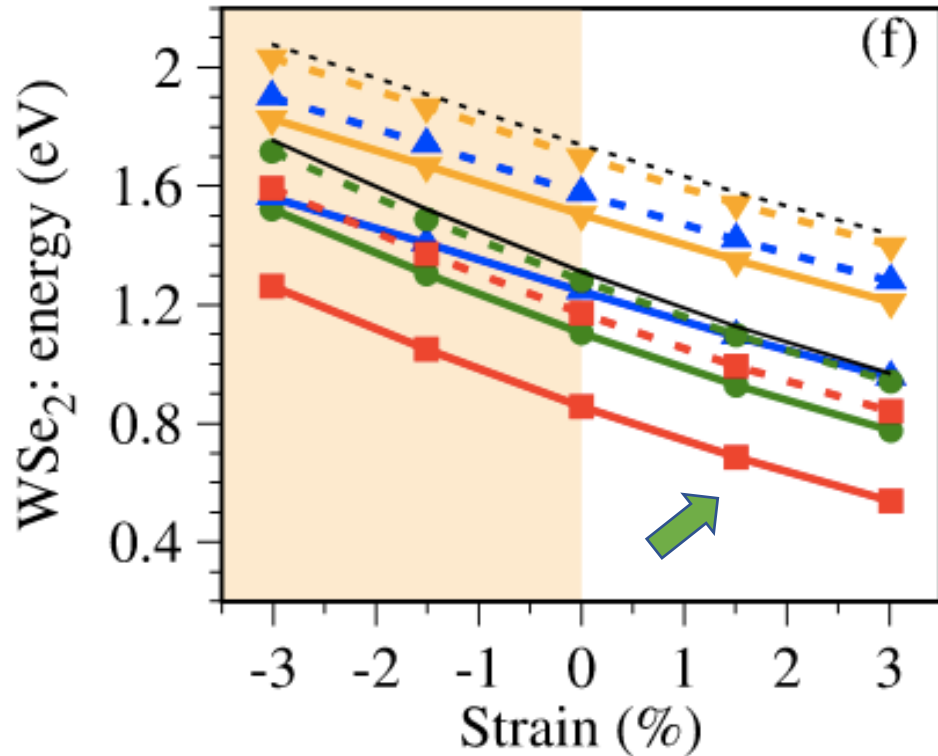
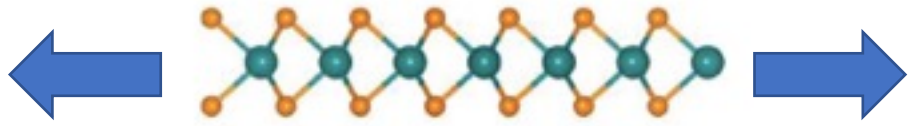
## Tensile strain



# Strain engineering in 2D materials

Zollner, K., Junior, P. E. F., & Fabian, J. (2019). Physical Review B, 100(19), 195126.

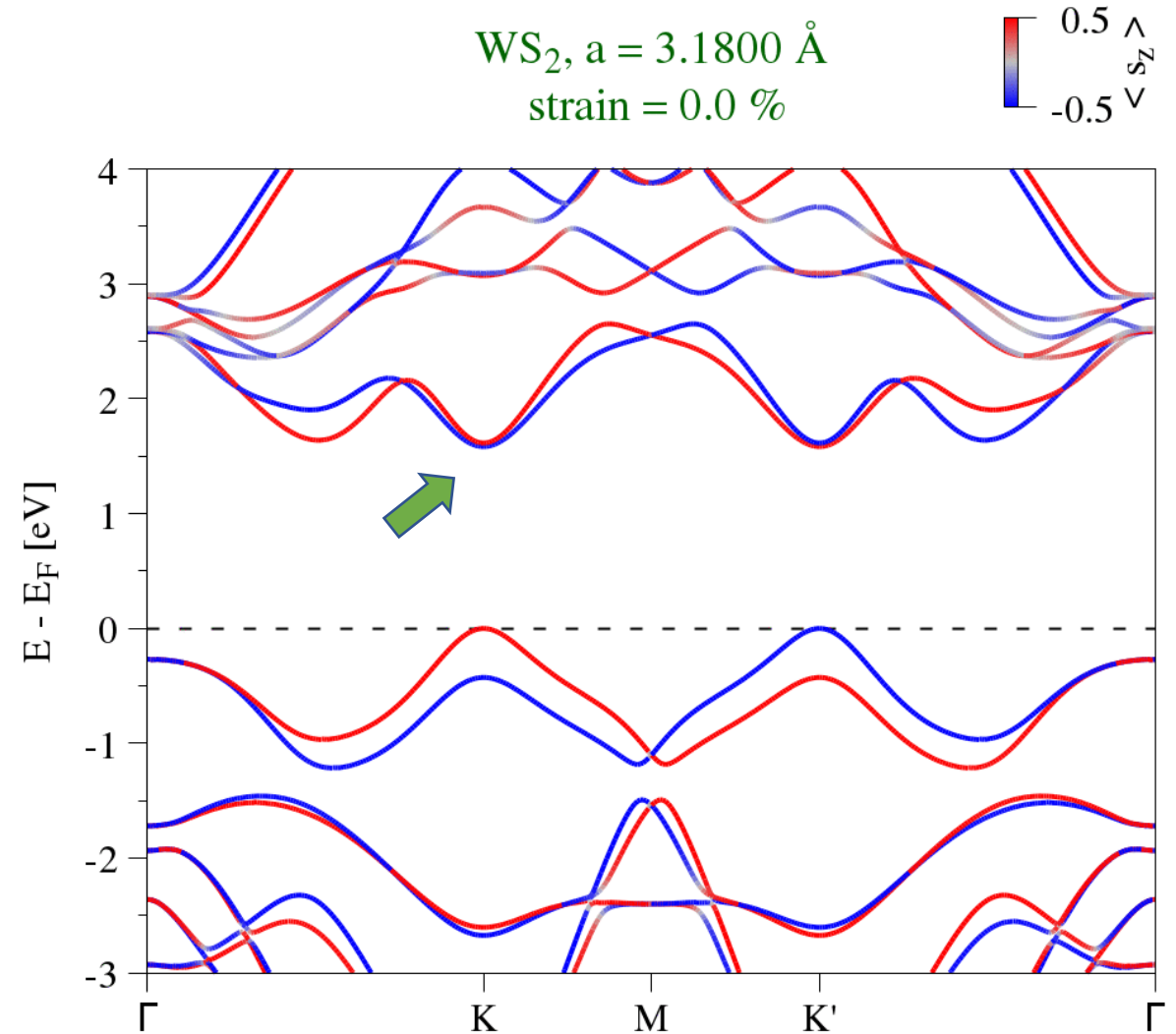
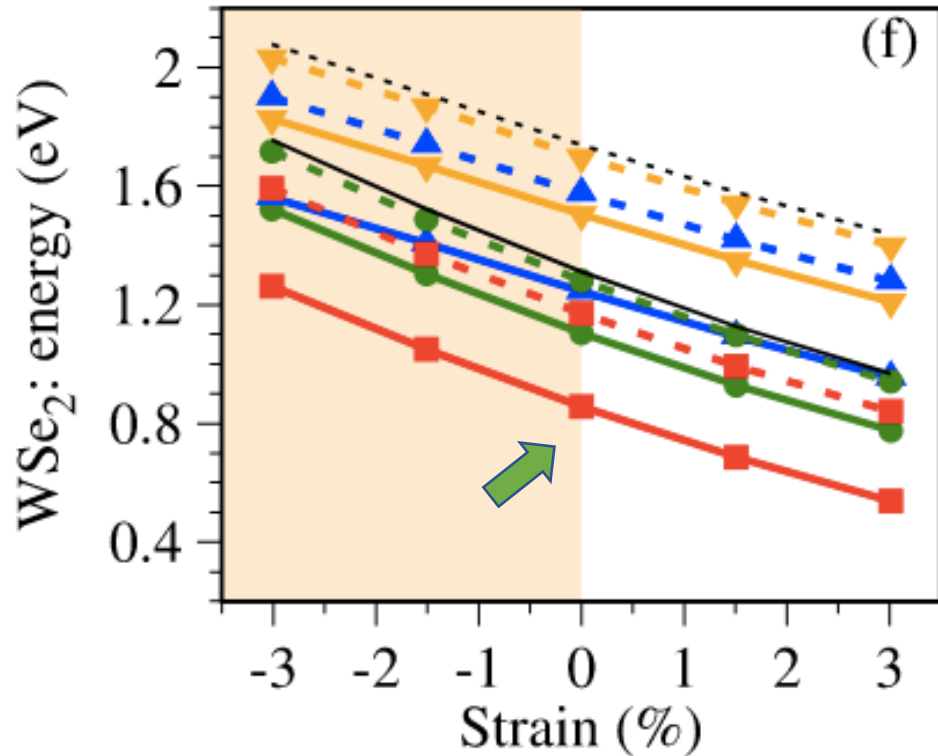
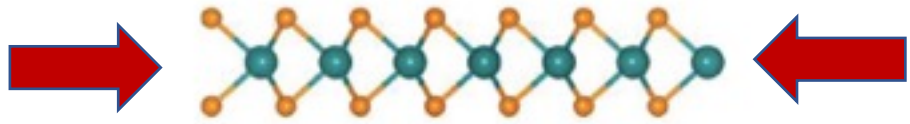
## Tensile strain



# Strain engineering in 2D materials

Zollner, K., Junior, P. E. F., & Fabian, J. (2019). Physical Review B, 100(19), 195126.

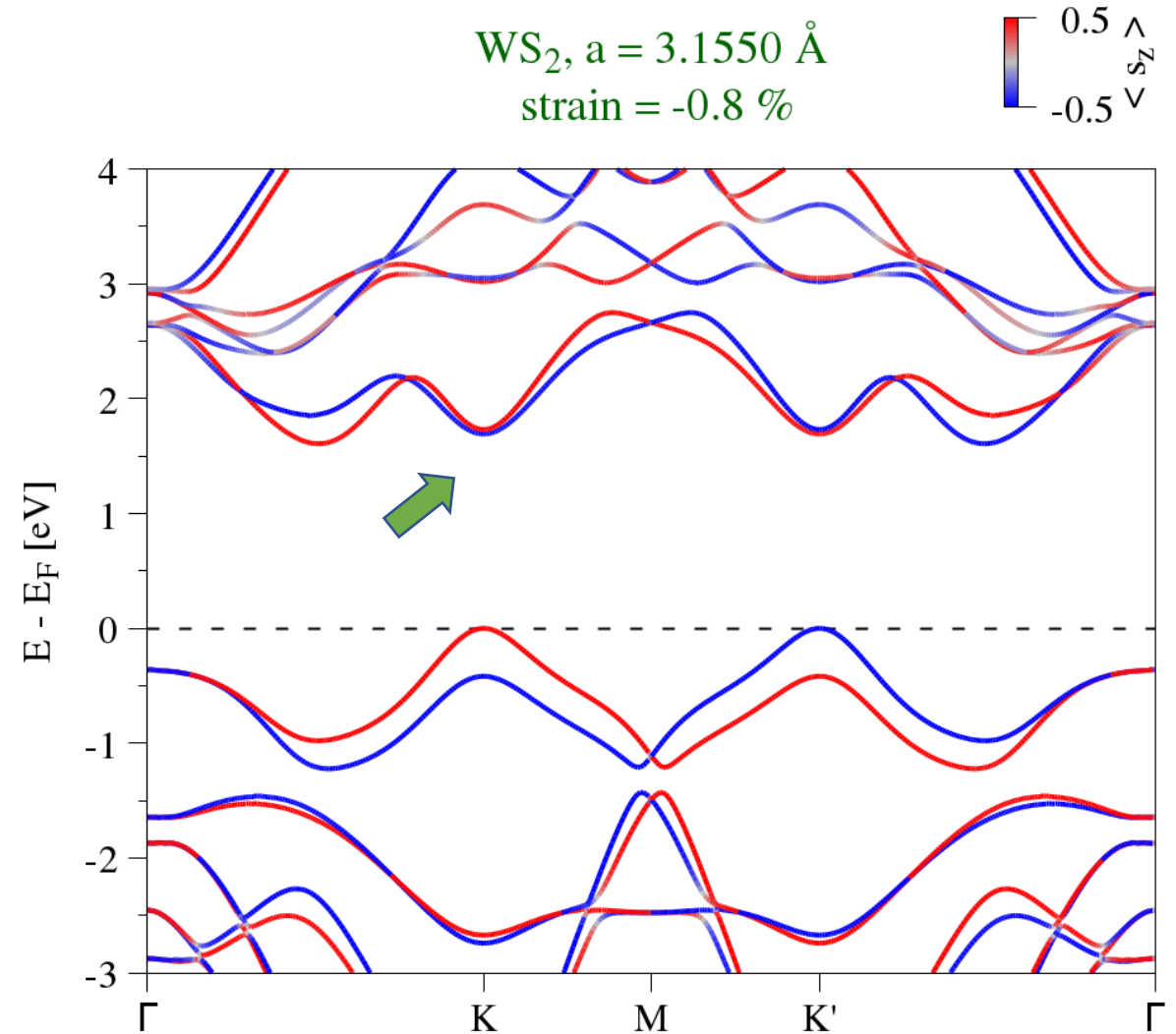
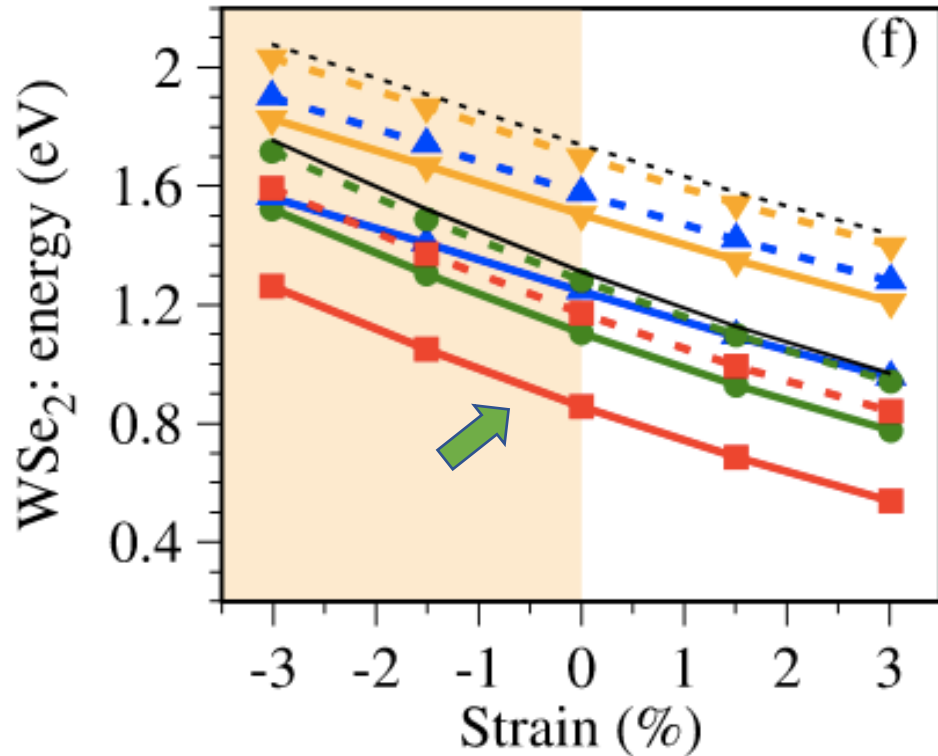
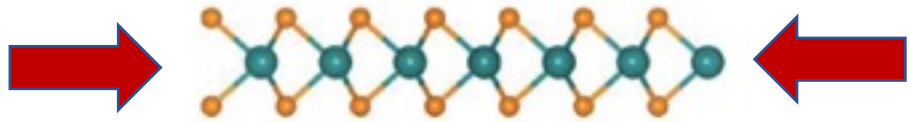
## Compressive strain



# Strain engineering in 2D materials

Zollner, K., Junior, P. E. F., & Fabian, J. (2019). Physical Review B, 100(19), 195126.

## Compressive strain

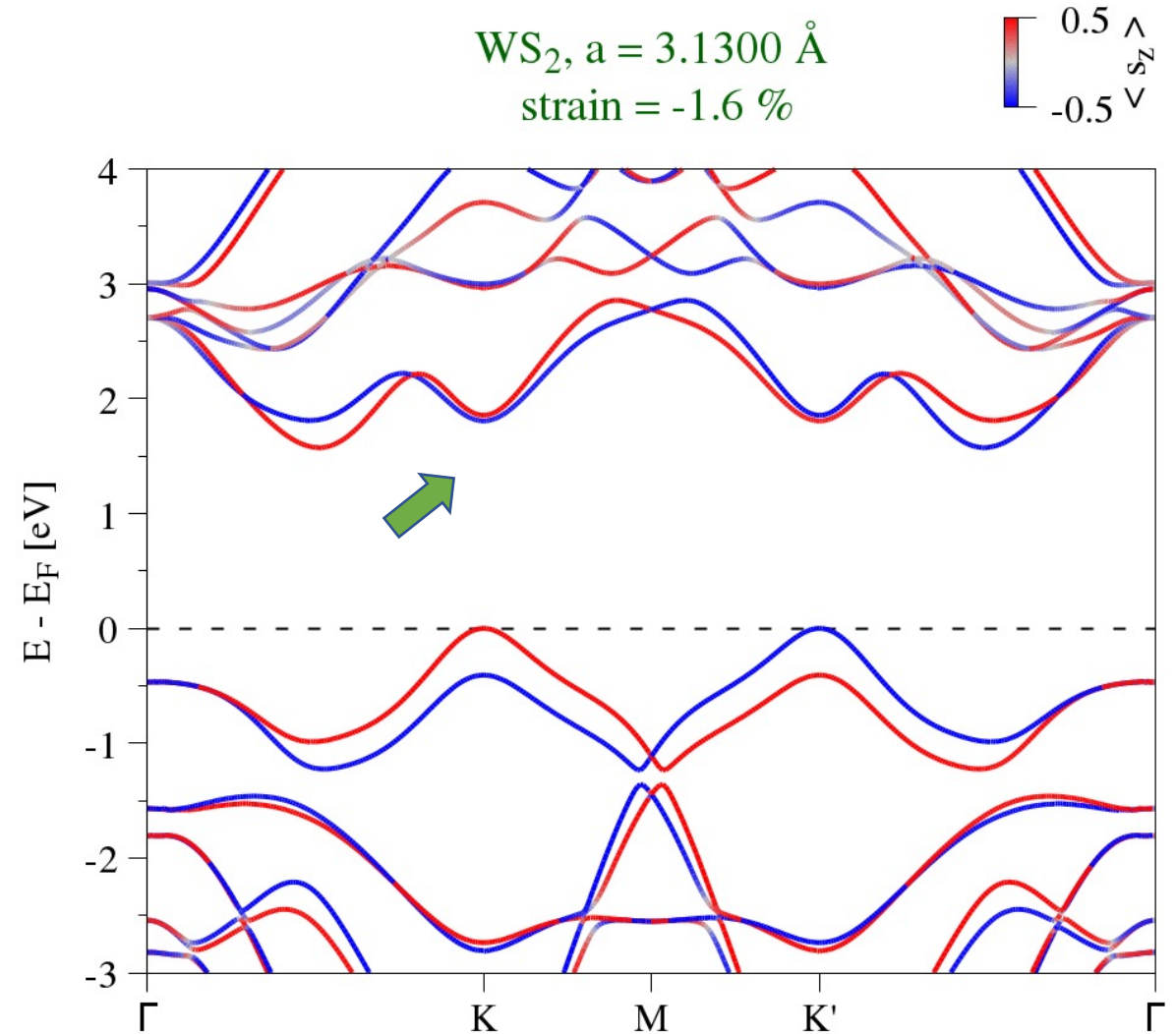
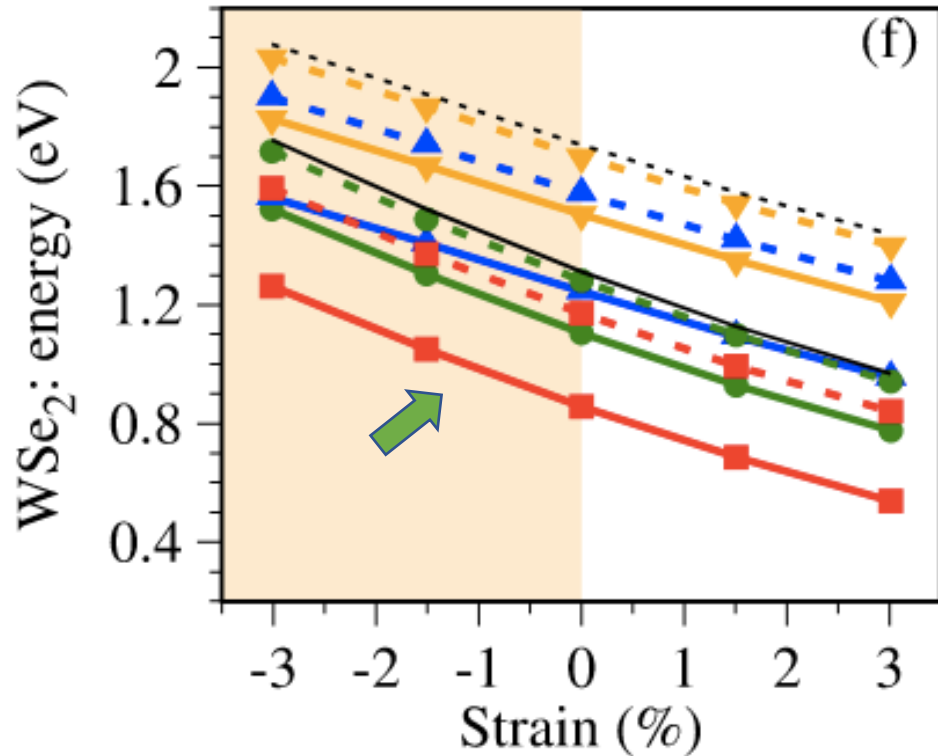
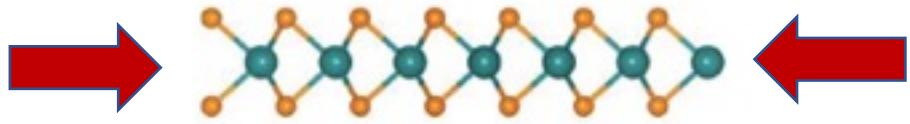




# Strain engineering in 2D materials

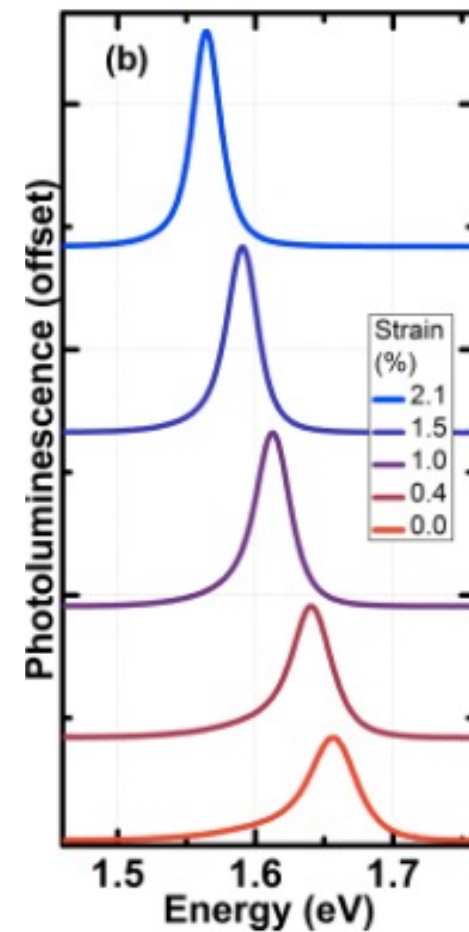
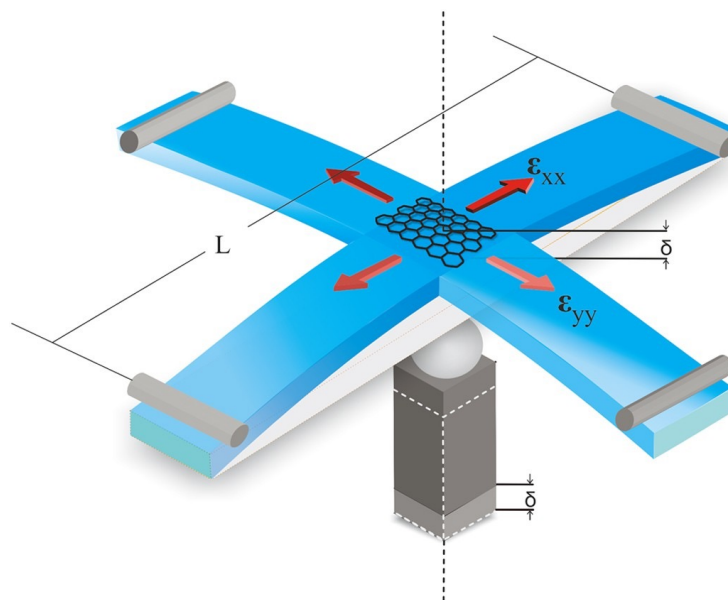
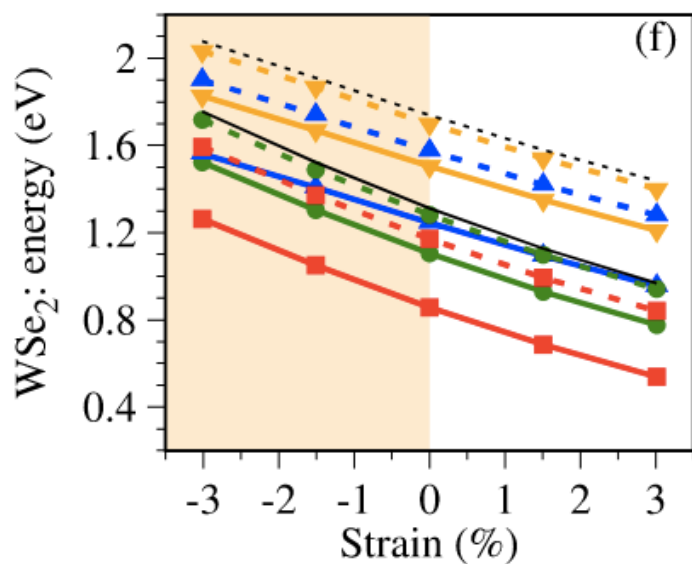
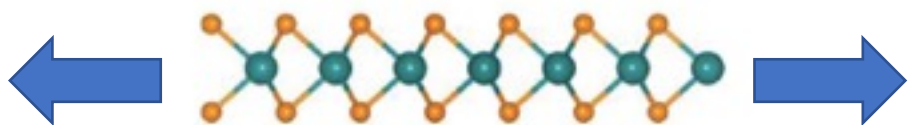
Zollner, K., Junior, P. E. F., & Fabian, J. (2019). Physical Review B, 100(19), 195126.

## Compressive strain



# Strain engineering in 2D materials

Tensile strain

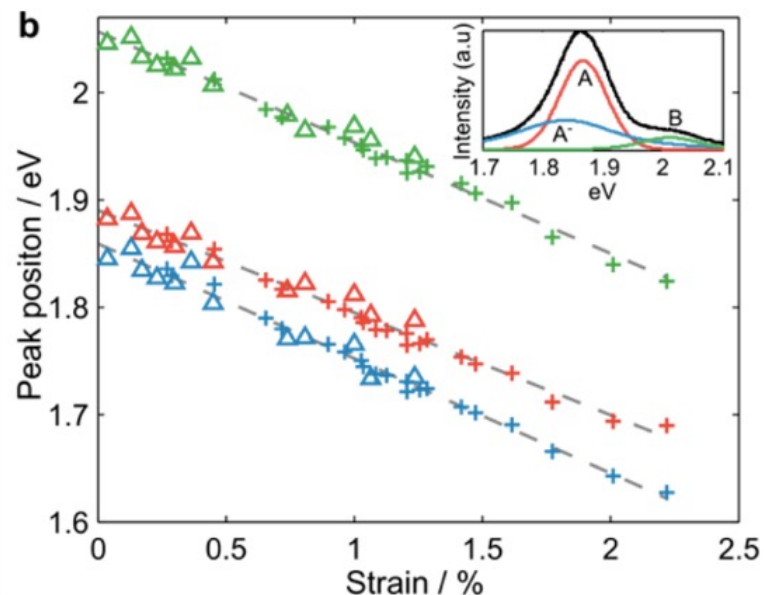
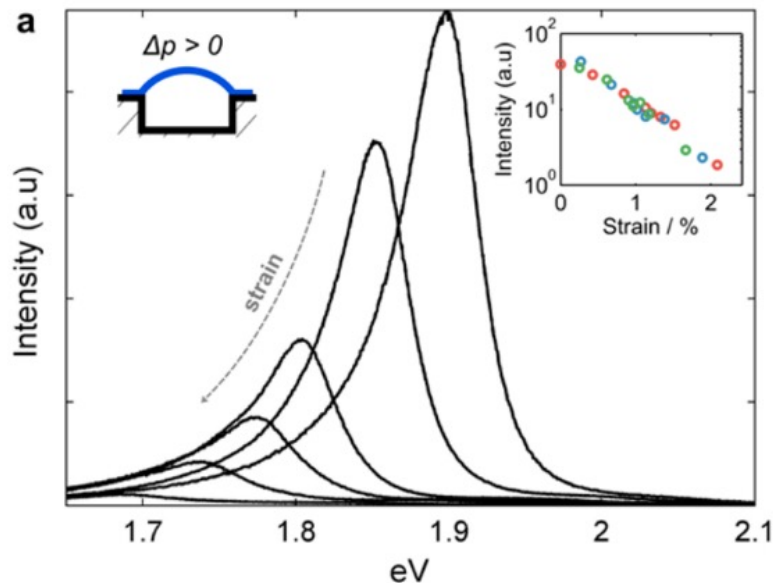
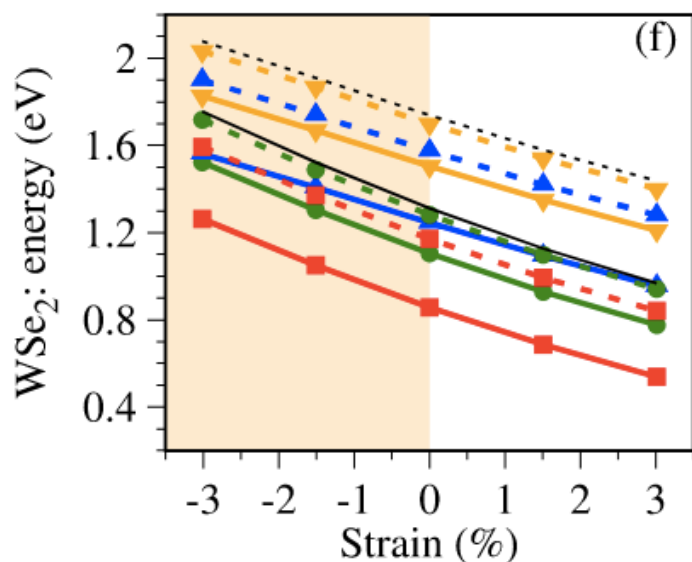
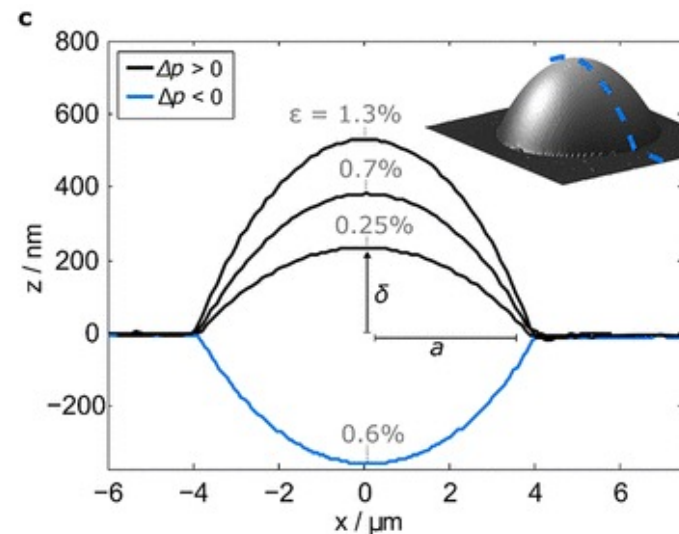
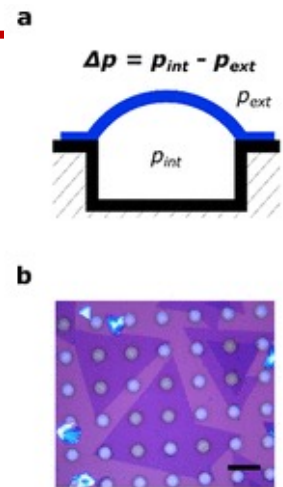
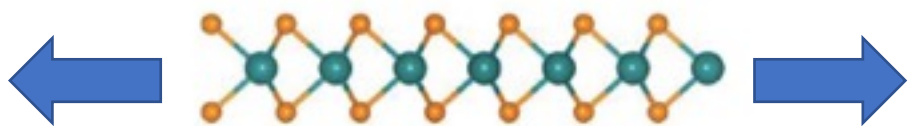


Aslan et al. PRB 98,115308 (2018)

Lloyd et al. Nano Lett. 2016, 16, 5836–5841

# Strain engineering in 2D materials

Tensile strain

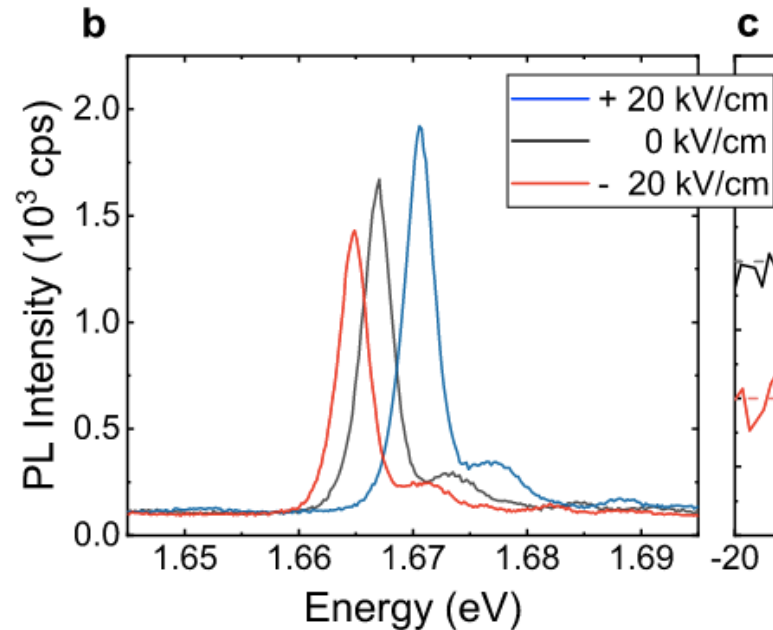
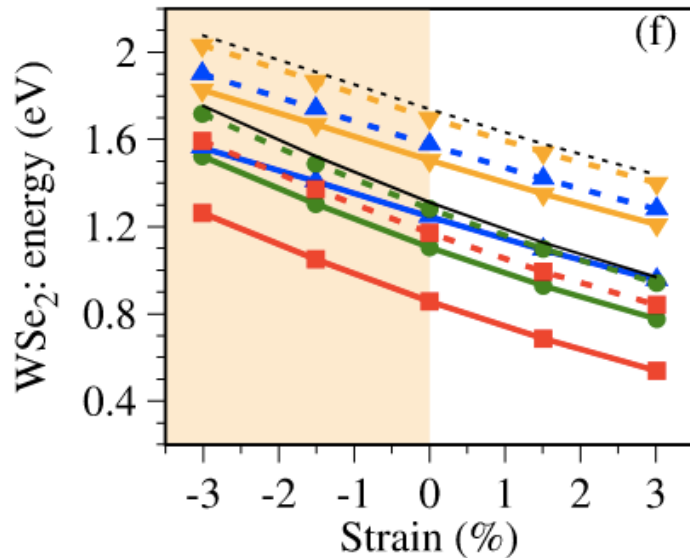
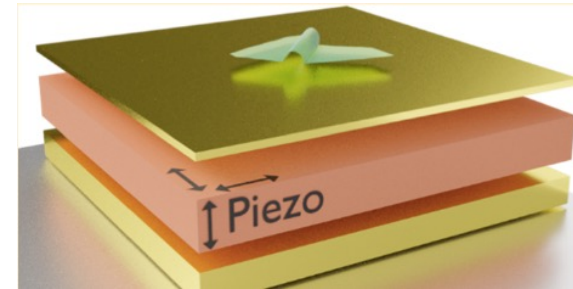
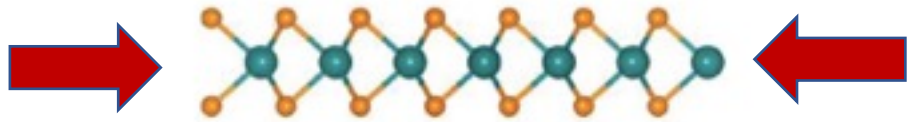


Aslan et al. PRB 98,115308 (2018)

Lloyd et al. Nano Lett. 2016, 16, 5836–5841

# Strain engineering in 2D materials

## Compressive strain

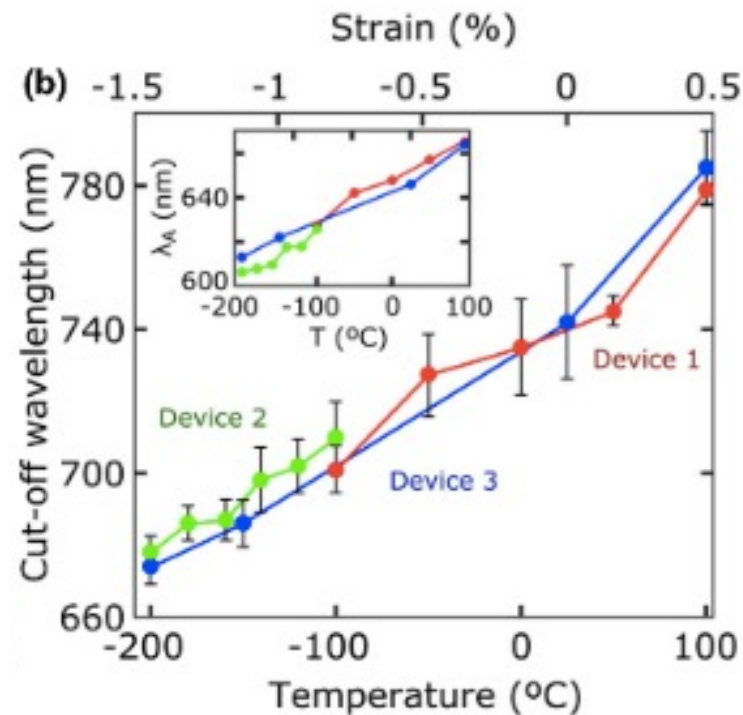
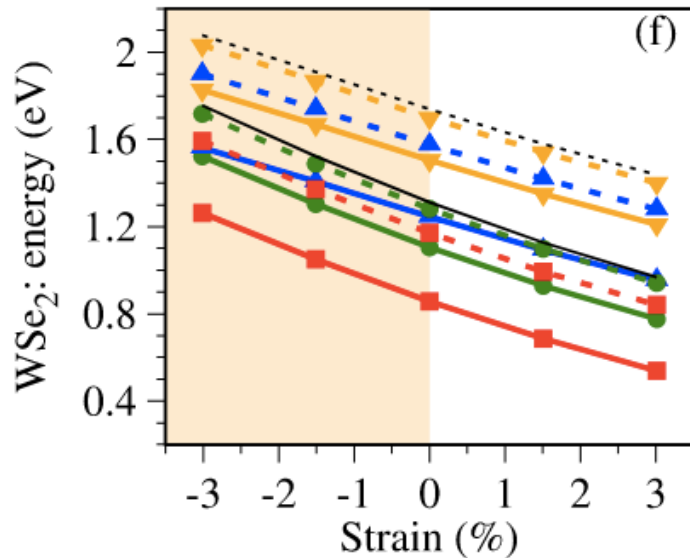
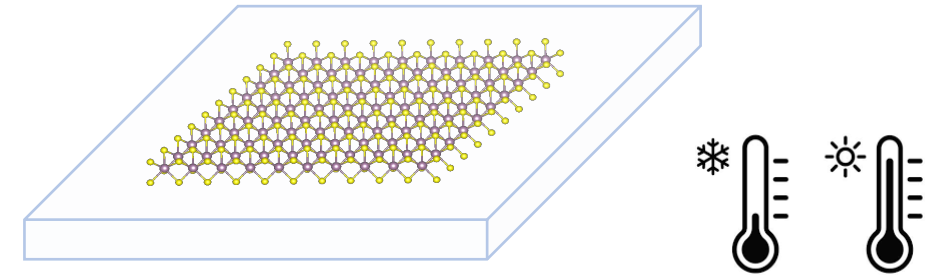
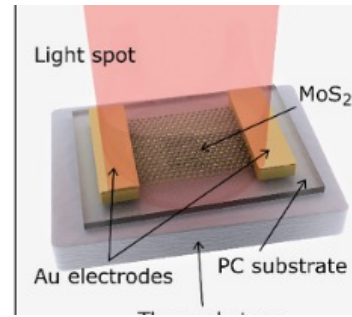
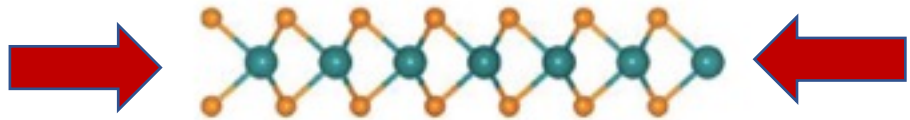


## Piezo actuators

- Small amounts of compressive strain
- Suitable for low temperature studies

# Strain engineering in 2D materials

## Compressive strain



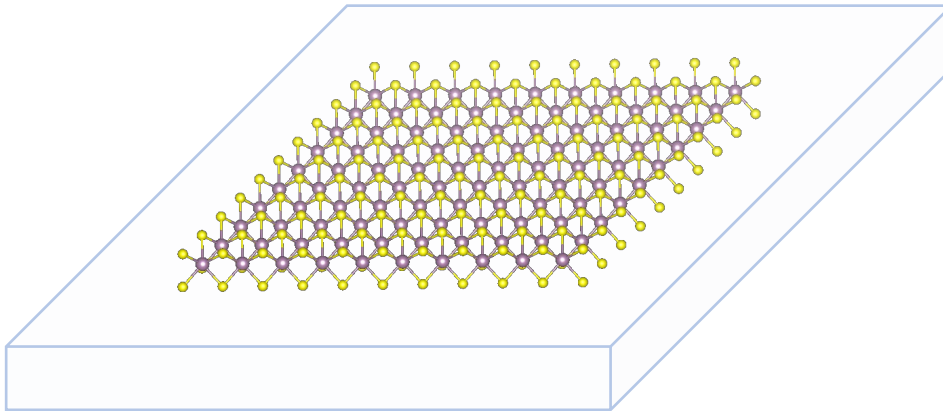
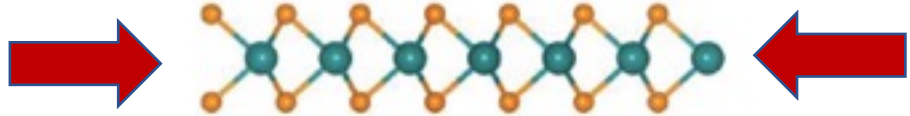
## Thermal expansion of Polymeric substrates:

- Large thermal coefficient
- Large Young modulus
- **Expansion up to 100C**
- **Compression down only to 80K**

# Thermal compression at lower temperatures

---

## Compressive strain



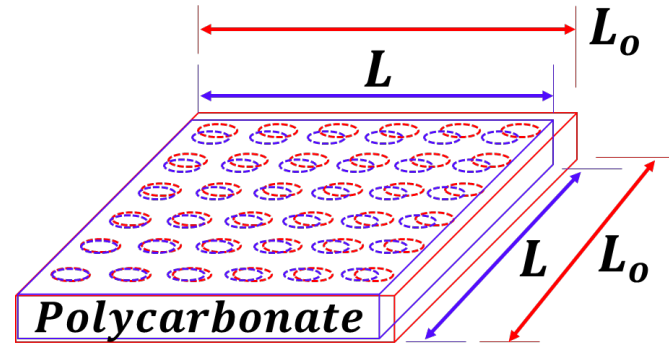
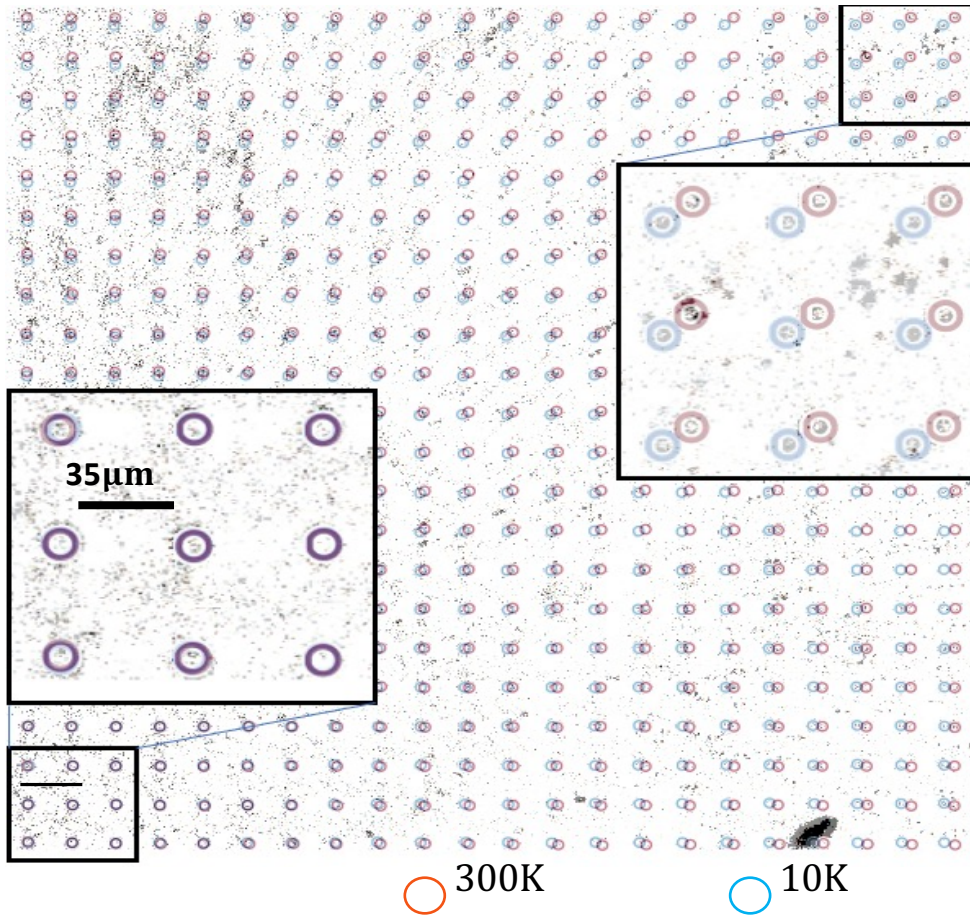
Would this work at lower  $T$ ?

Advantages:

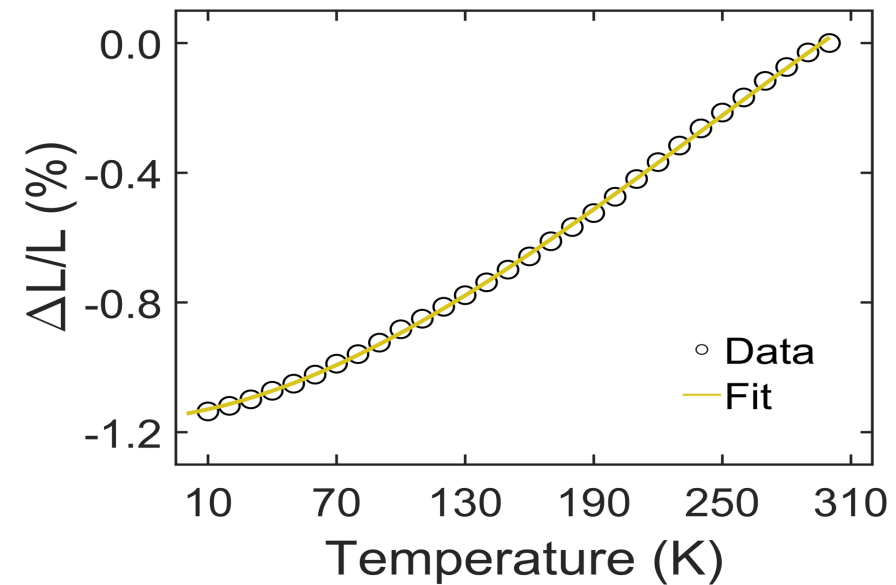
- ❖ Simple preparation
- ❖ Large biaxial compressive strain
- ❖ Low temperature phenomena

# Polycarbonate substrate deformation

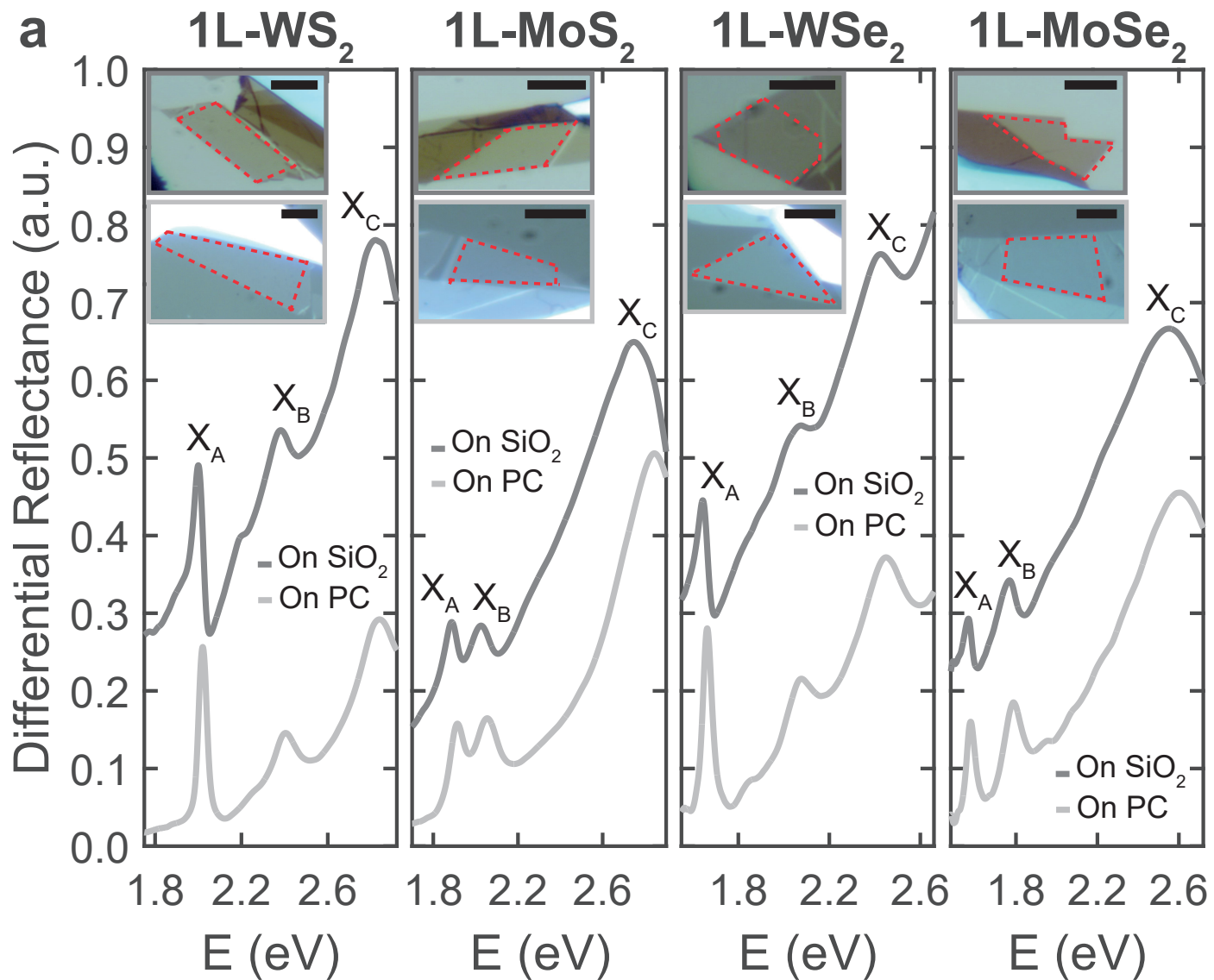
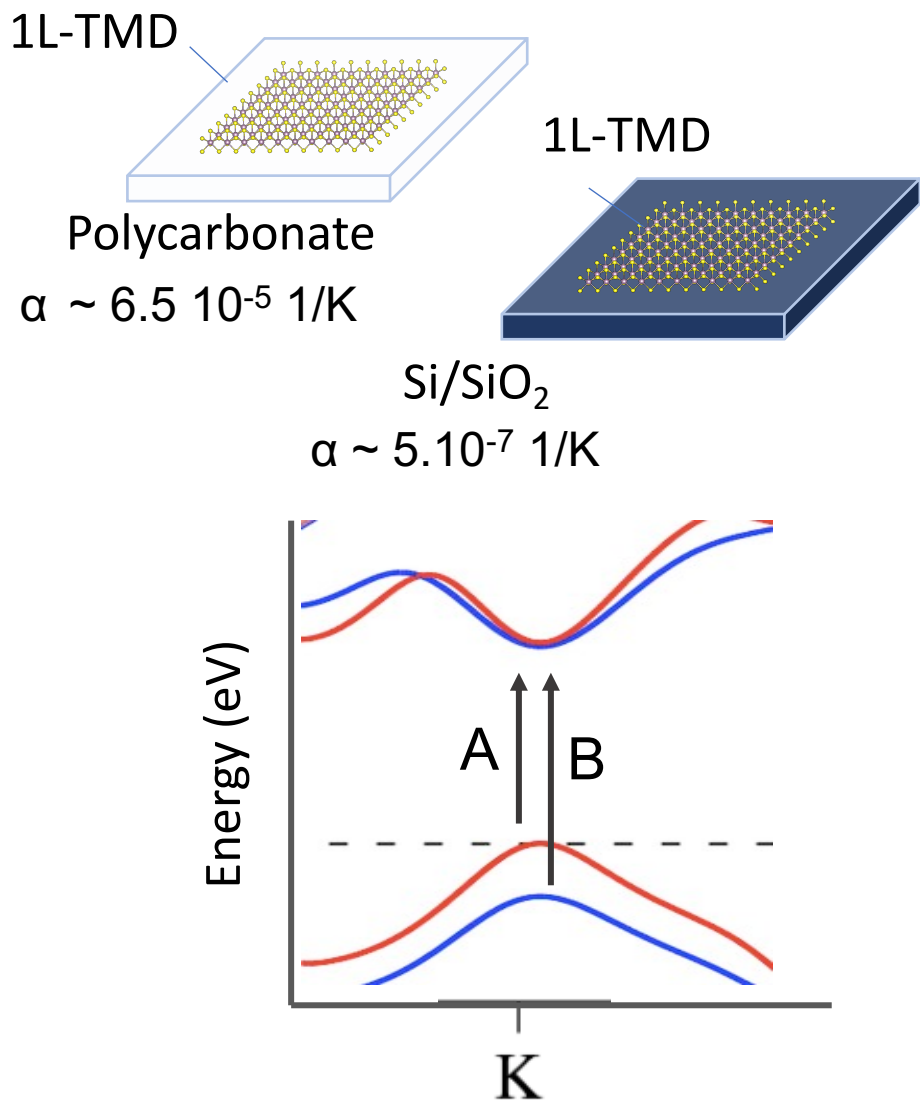
$$\alpha \sim 6.5 \cdot 10^{-5} \text{ 1/K}$$



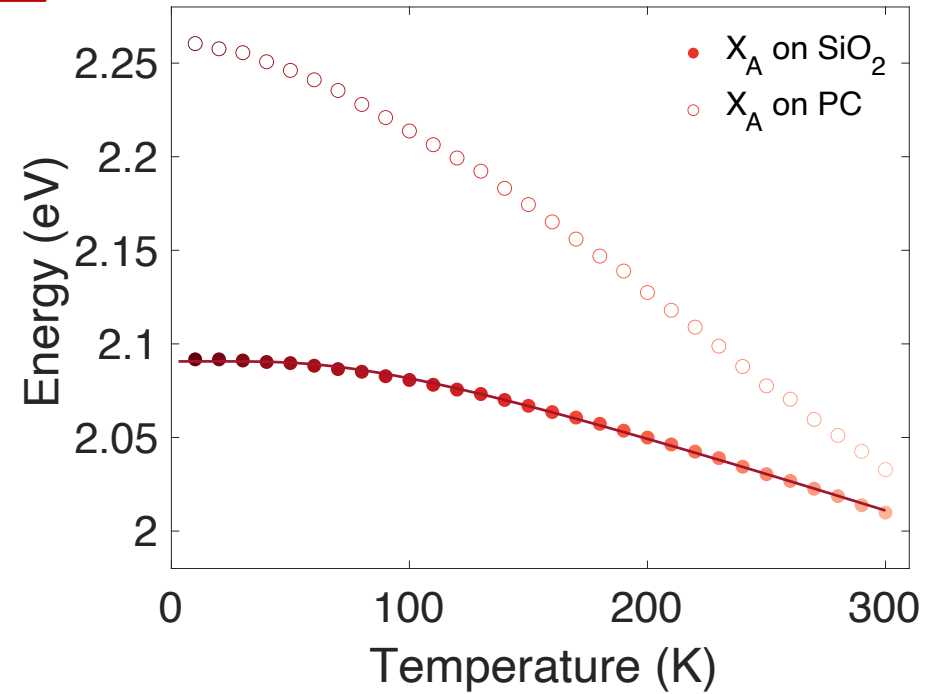
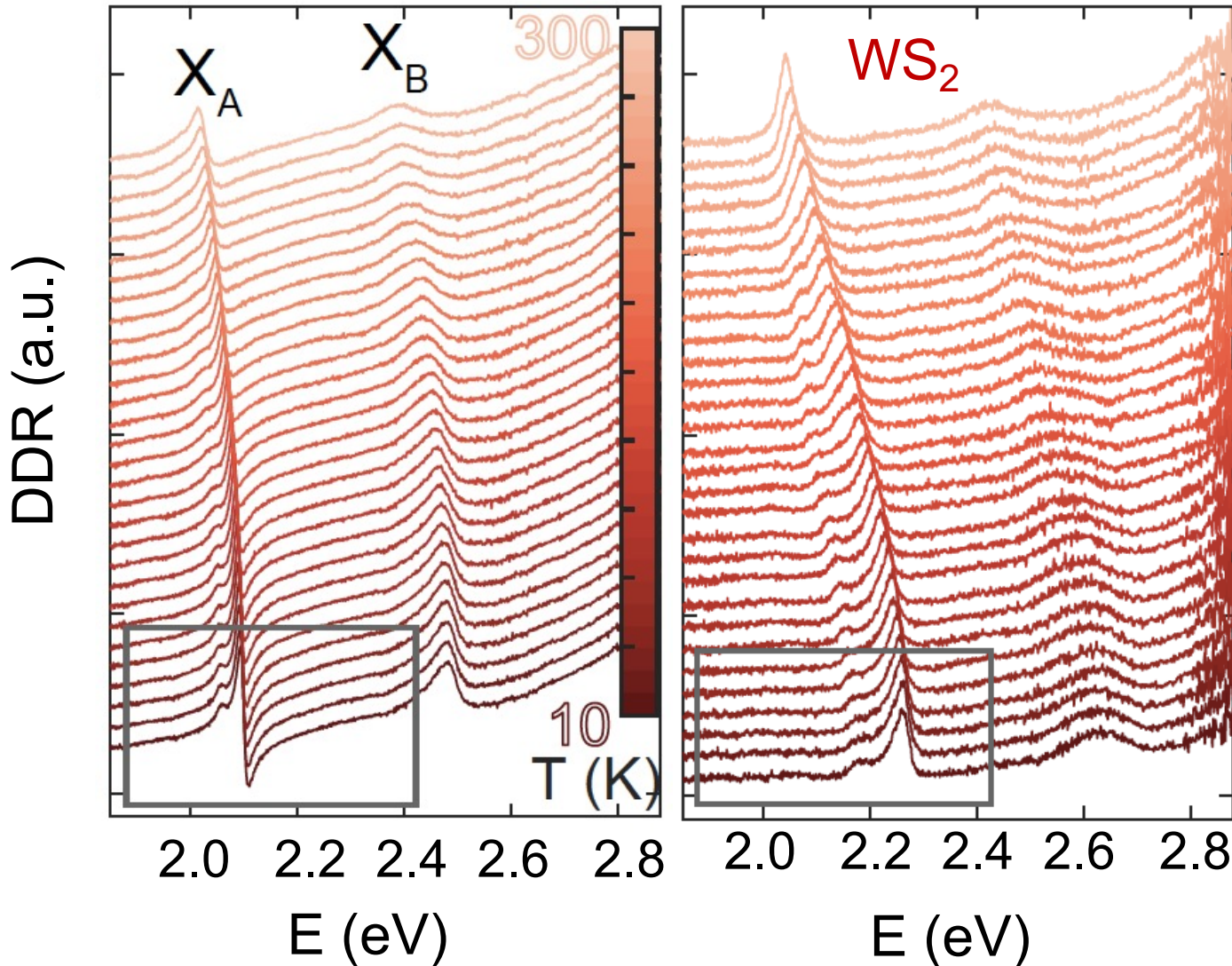
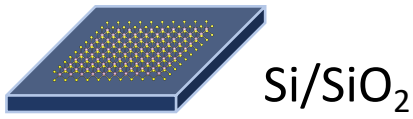
$$\frac{\Delta L}{L} (\%) = \frac{L - L_0}{L_0} 100\%$$



$$\frac{\Delta L}{L} (T) = aT^3 + bT^2 + cT + d$$

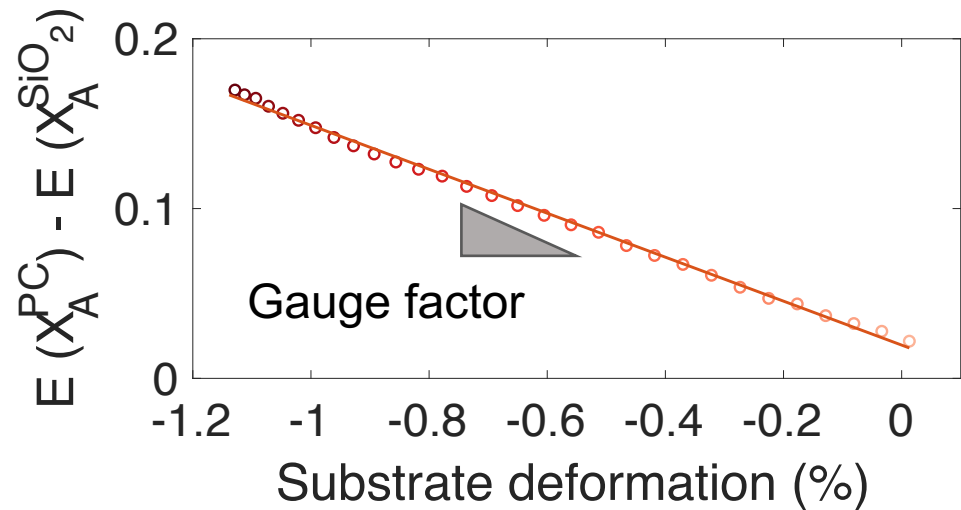
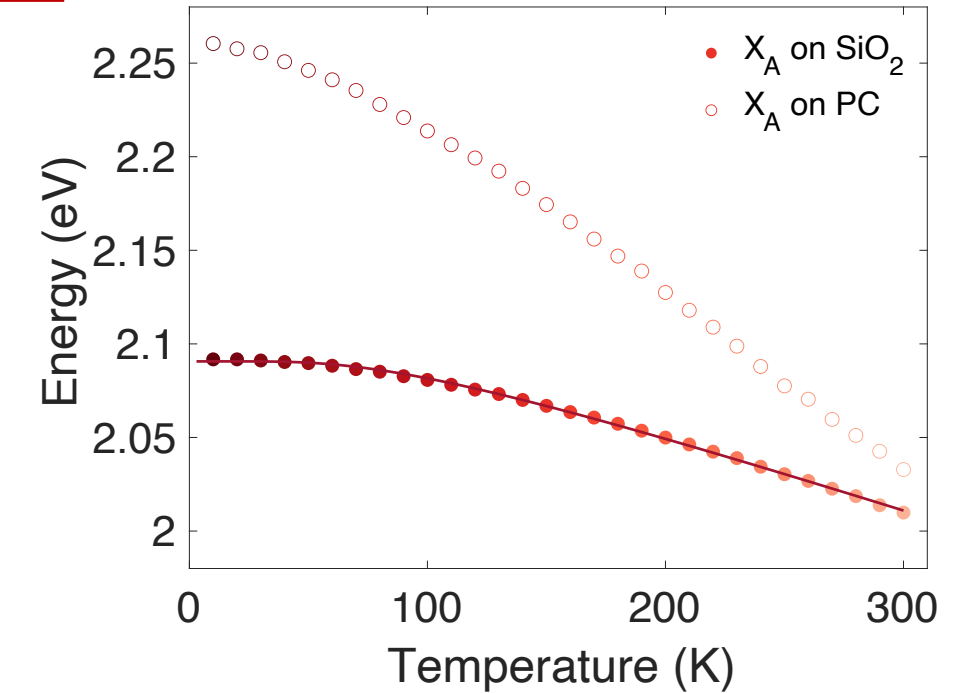
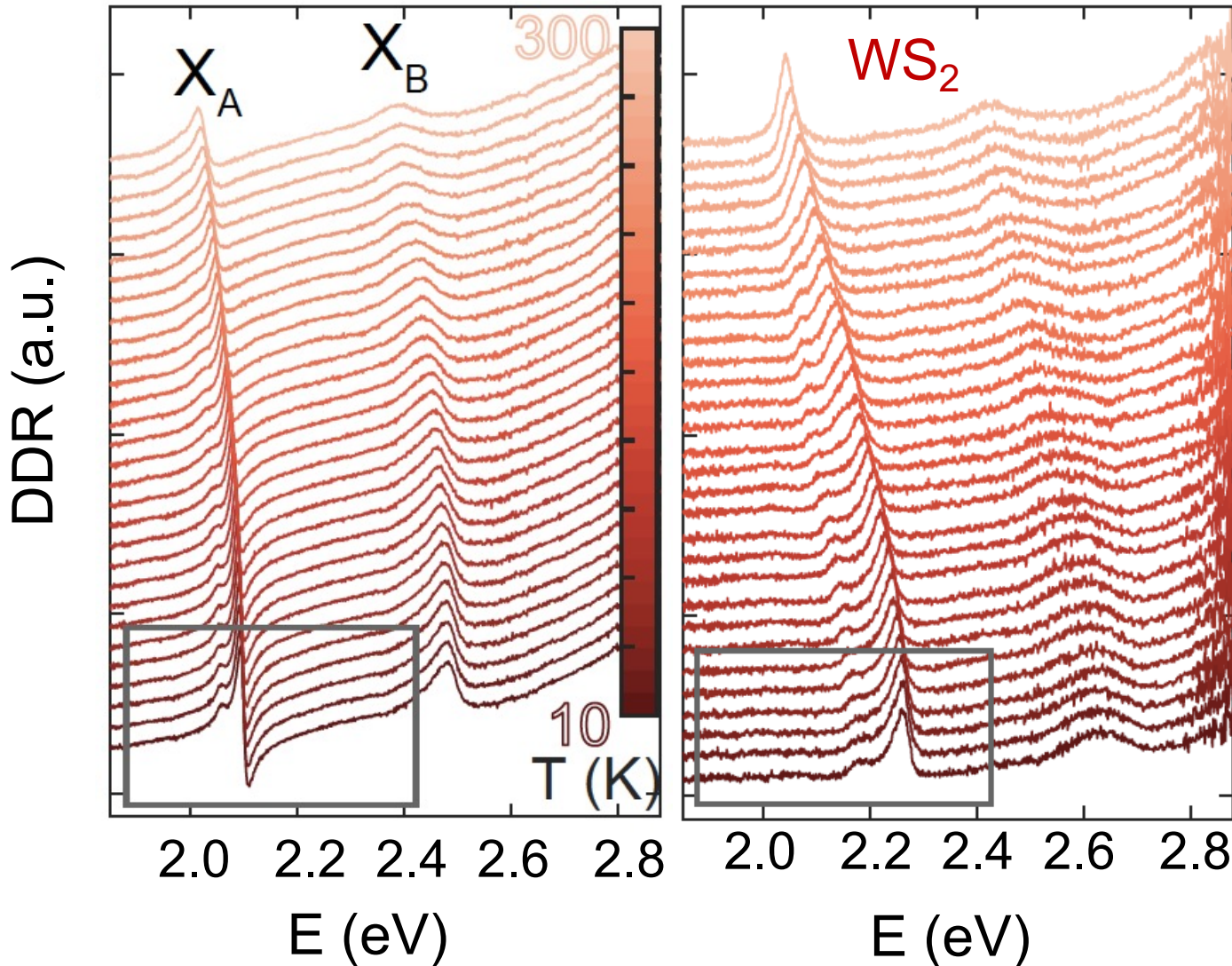
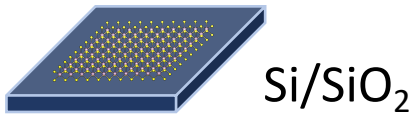




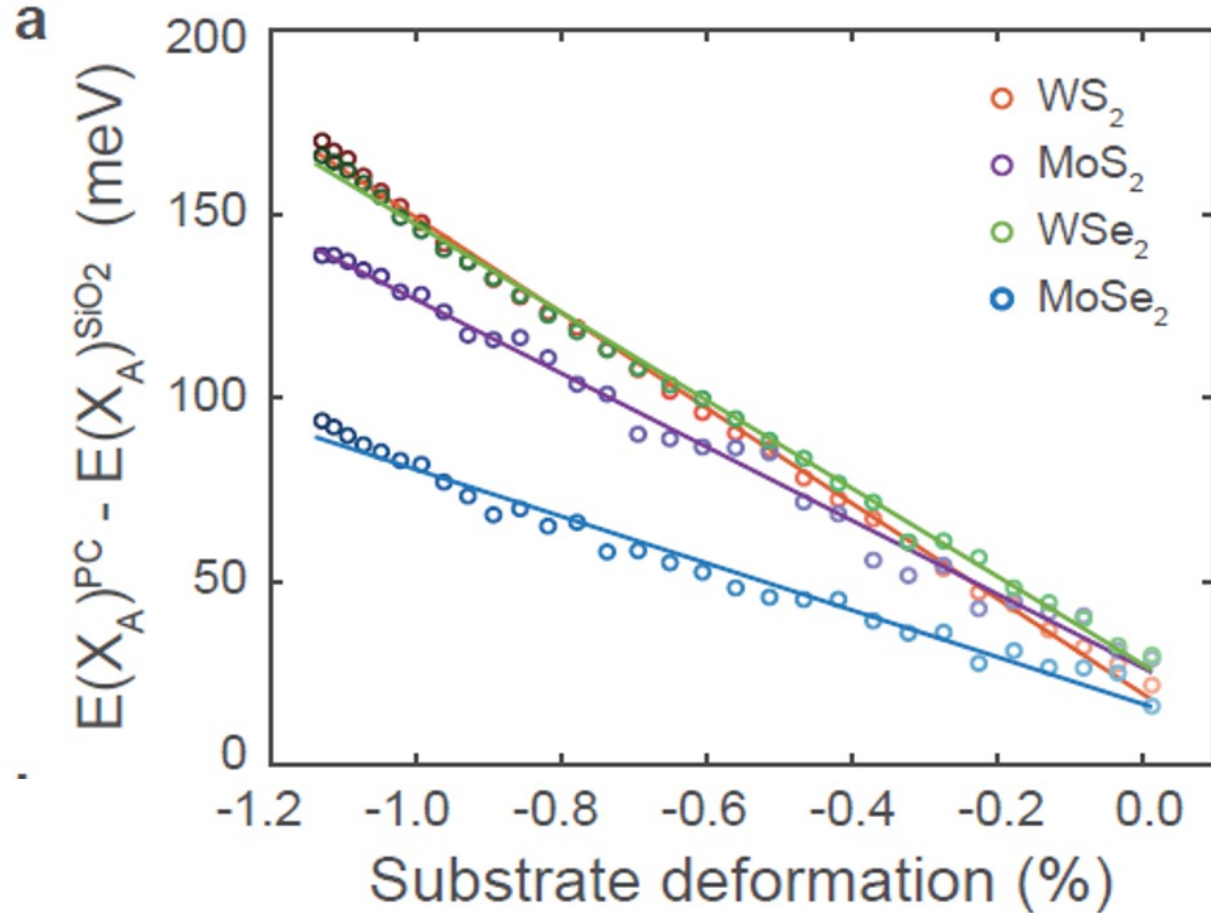


$$E_g(T) = E_g(0) - S \langle \hbar\omega \rangle [ \coth(\langle \hbar\omega \rangle / 2kT) - 1 ]$$

O'Donnell et al Appl. Phys. Lett. 58, 2924 (1991)



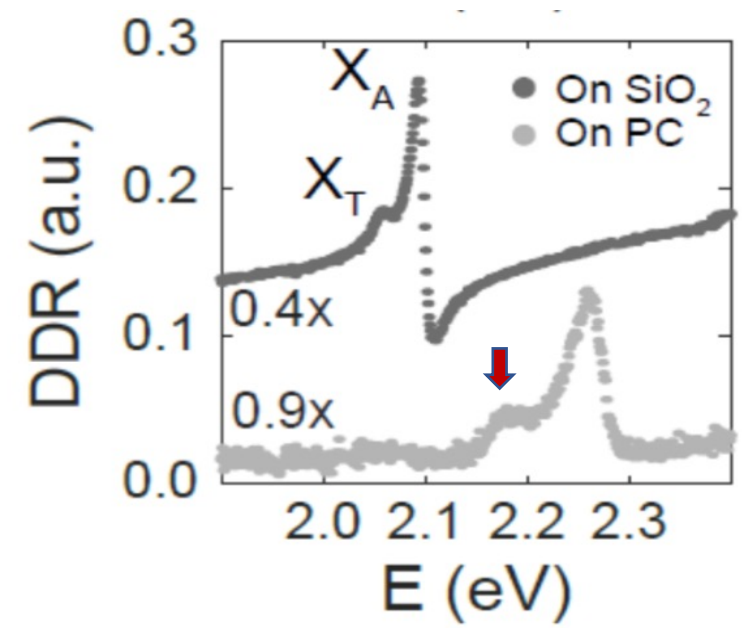
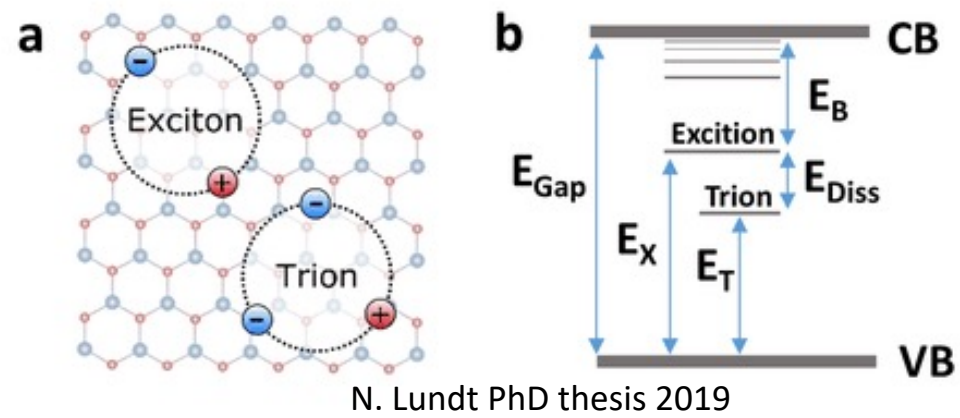
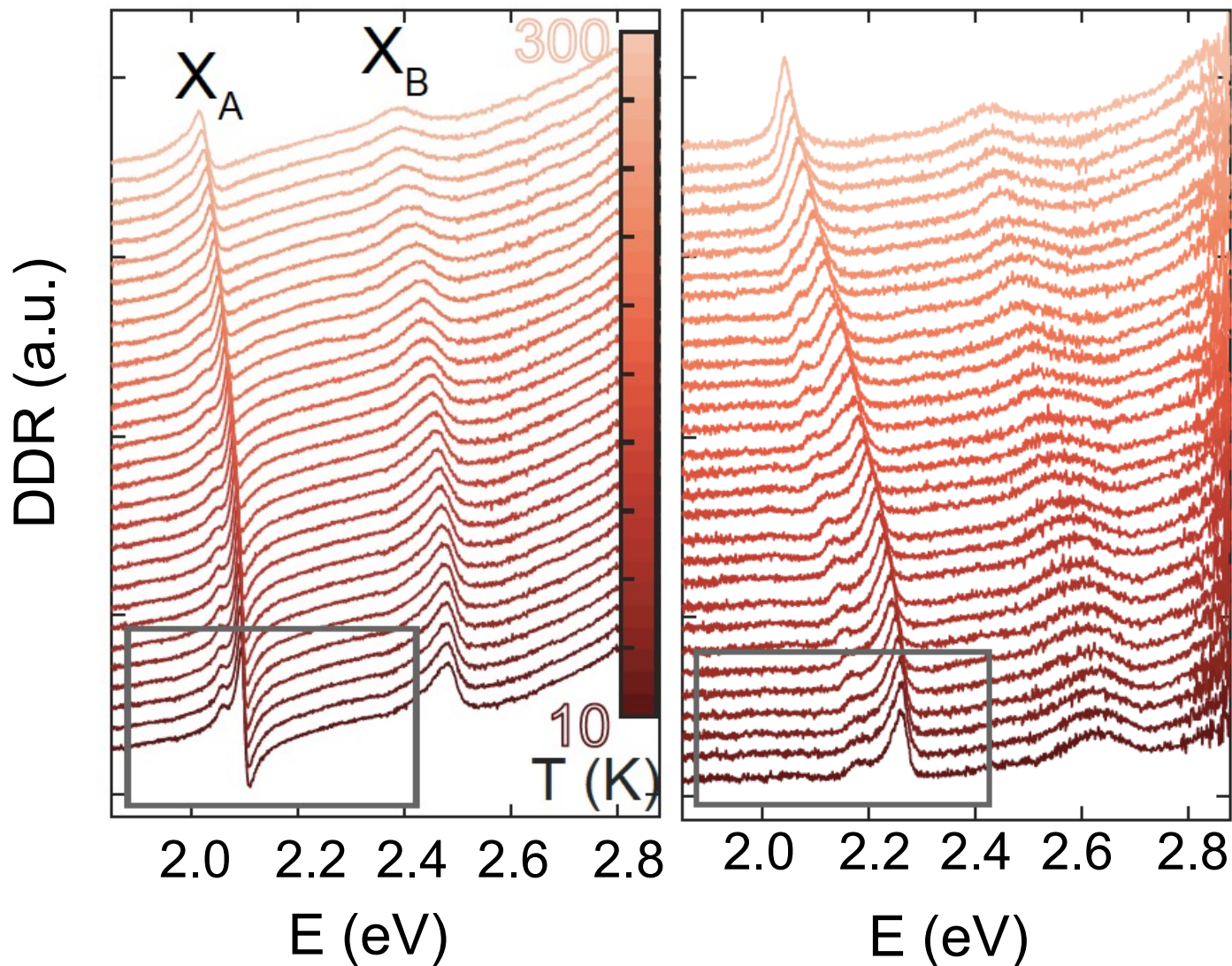
27 Strain gauge factors for excitons



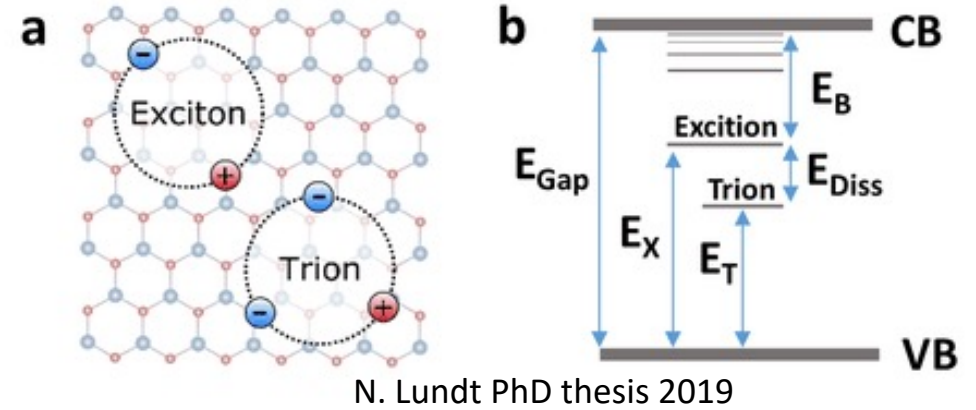
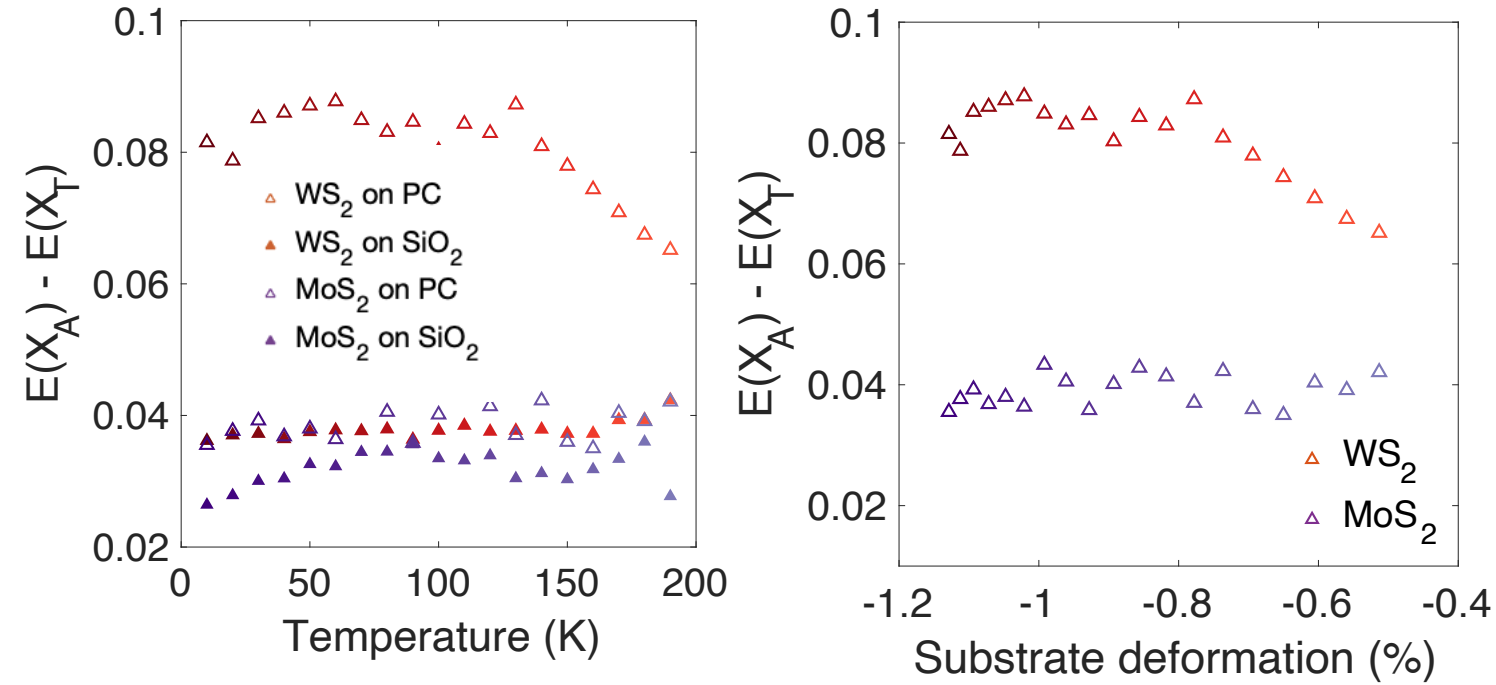
Gauge factor (meV/%)	$X_A$ This work	$X_A$ Theory	$X_B$ This work	$X_B$ Theory
1L- $WS_2$	<b><math>-129 \pm 3</math></b>	$-151^1$ $-144.0^2$	$-112 \pm 10$	$-130^1$ $-123.8^2$
1L- $MoS_2$	$-100 \pm 3$	$-110^1$ $-112.5^2$	$-90 \pm 5$	$-107^1$ $-109.8^2$
1L- $WSe_2$	$-120 \pm 3$	$-134^1$ $-131.2^2$	$-129 \pm 10$	$-111^1$ $-109.7^2$
1L- $MoSe_2$	$-64 \pm 4$	$-90^1$ $-98.6^2$	$-66 \pm 4$	$-89^1$ $-97.2^2$

1: Frisenda, NPJ 2D materials,2017 2: Zollner,PRB, 2019

- Very good strain transfer
- Unprecedented amount of biaxial compressive strain ( $\sim 1.2\%$ )



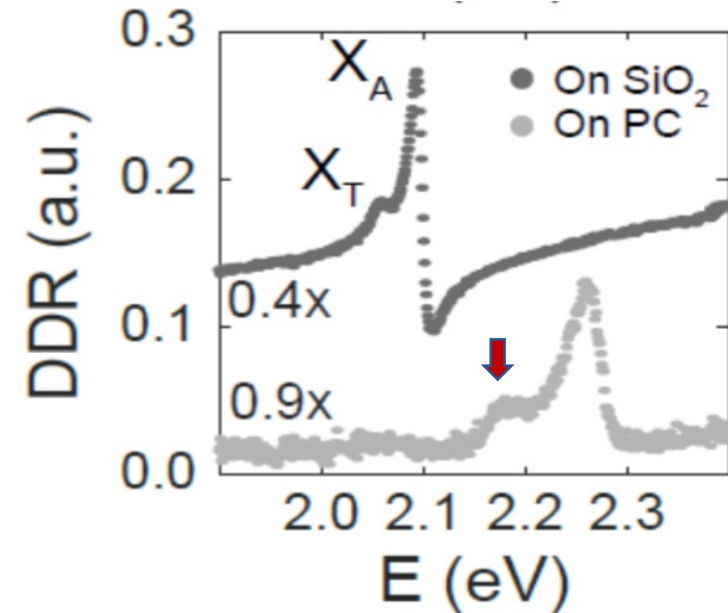
29 Micro-reflectance spectroscopy



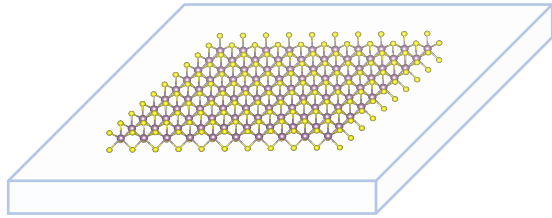
$E_b(X_T)$ (meV)	on $SiO_2$	On PC
$MoS_2$	~25	~40
$WS_2$	~40	~80

Binding energies for exciton and trions depend on

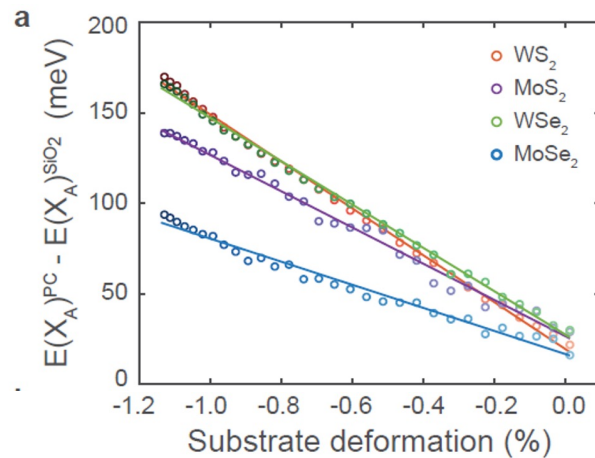
- Effective masses
- Dielectric screening
- Doping levels



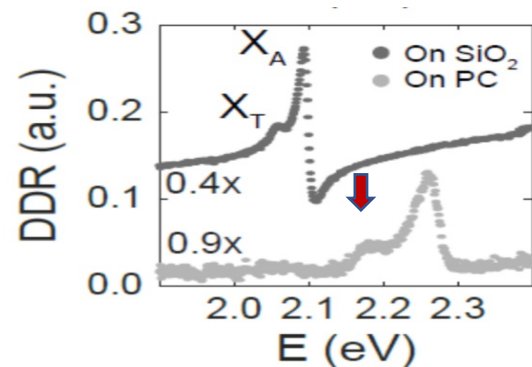
# Conclusions and outlook



- Thermal compression suitable methods to study effects of compressive biaxial strain in 2D materials



- Low temperature regime enables high spectroscopy resolution, allow study of excitonic complexes under strain: interest for valleytronics and exciton transport



- Strain engineering for many other quantum properties in low temperature phases: from phase transition to other quantum properties tuned or induced by strain



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