

# Optical properties of single-layer, double-layer, and bulk MoS<sub>2</sub>

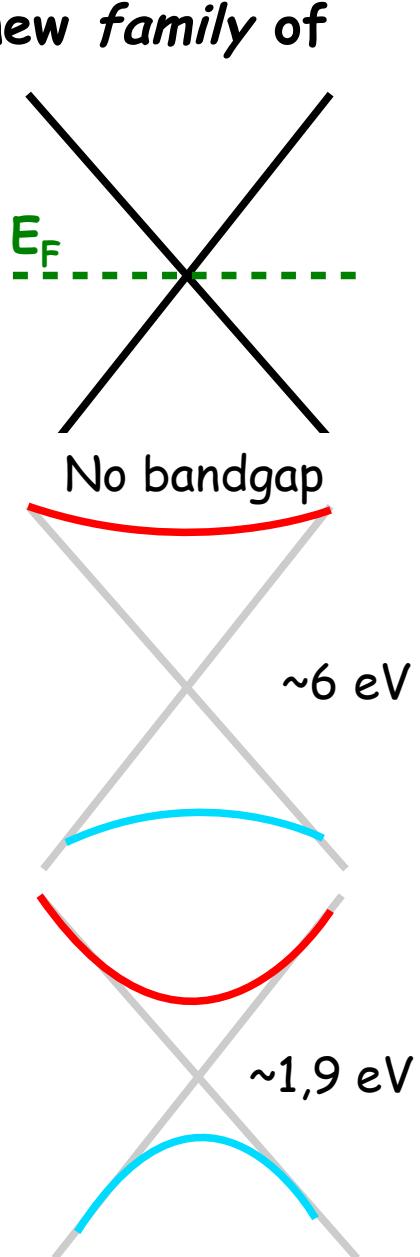
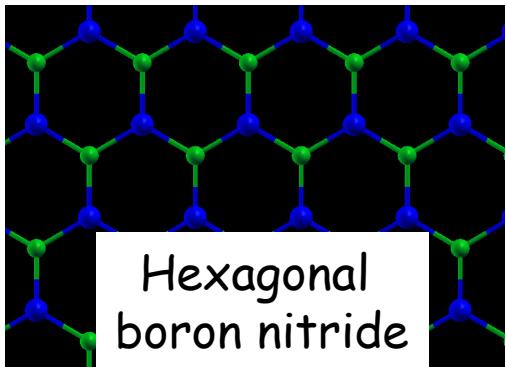
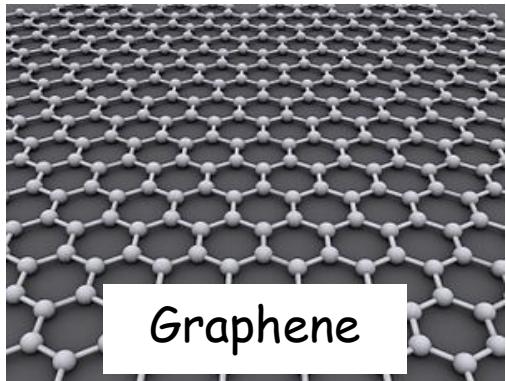
*Alejandro Molina-Sánchez, Ludger Wirtz,  
Davide Sangalli, Andrea Marini, Kerstin  
Hummer*



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Physics and Material Sciences  
Research Unit (PHYMS)

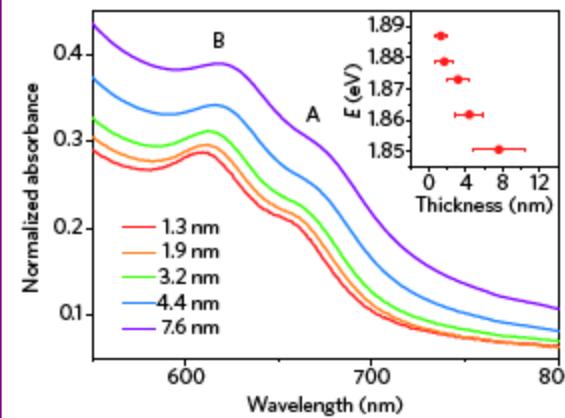
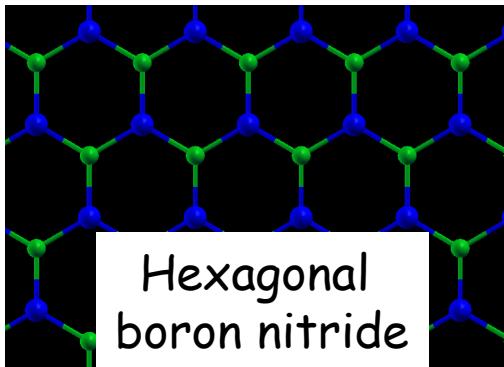
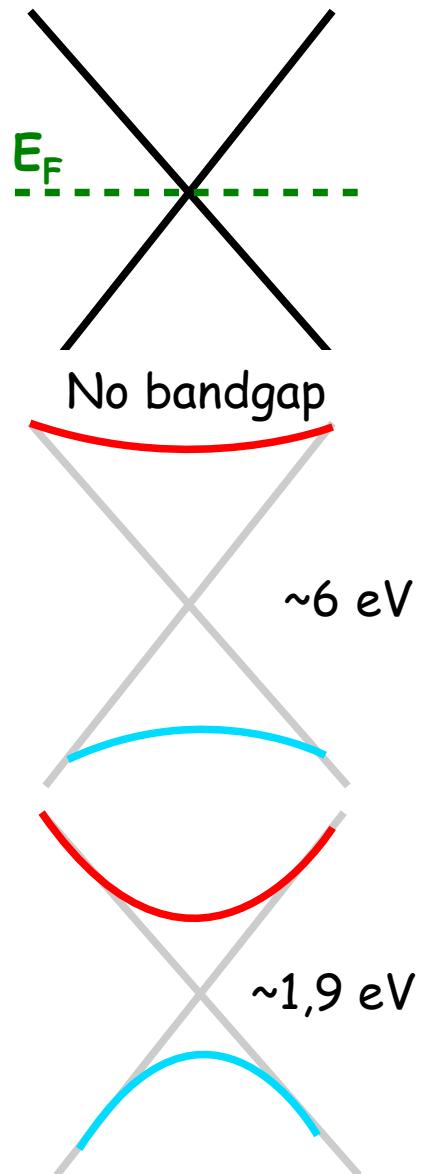
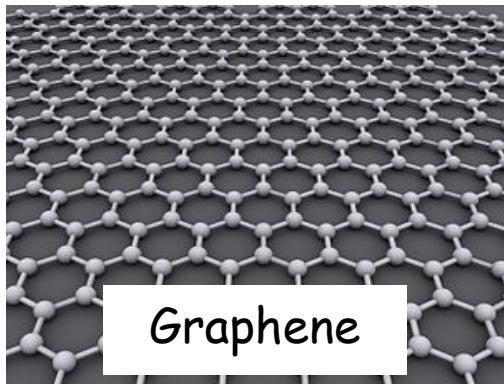
# Single-layer semiconductors

From graphene to a new family of materials

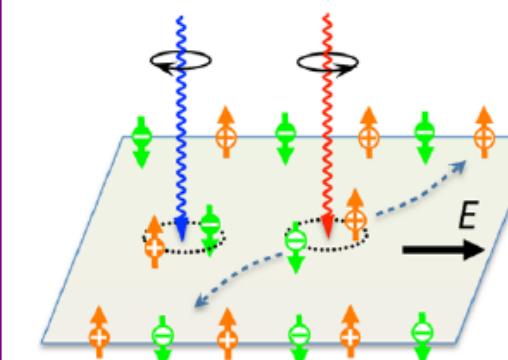
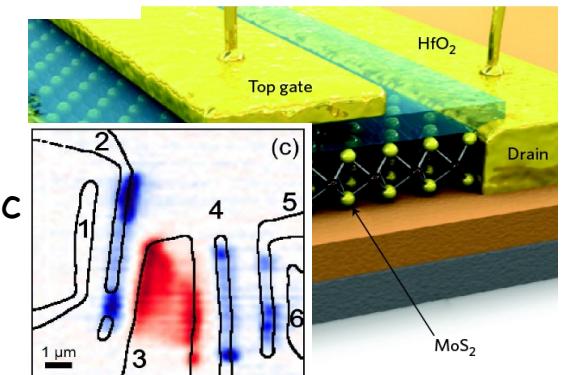


# Single-layer semiconductors

From graphene to a new *family* of materials



The bandgap and the high mobility makes MoS<sub>2</sub> a suitable alternative to graphene or carbon nanotubes.



Broad variety: MoSe<sub>2</sub>, WS<sub>2</sub>, MoSe<sub>2</sub>

See review Nature Nanotechnology 7, 699 (2012)

A. Castellanos, Nano Lett.,

Phys. Rev. Lett. 108, 196802 (2012)

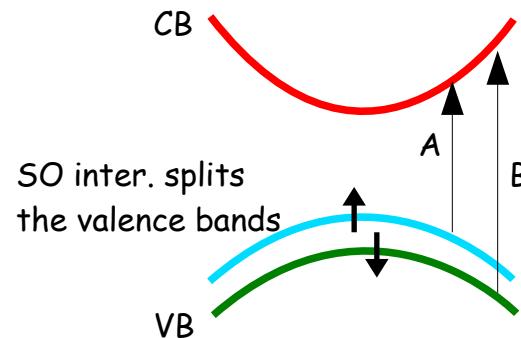
# Transition metal dichalcogenides

## Single-layer semiconductors

Crystal symmetry  
determines the  
electronic  
structure and  
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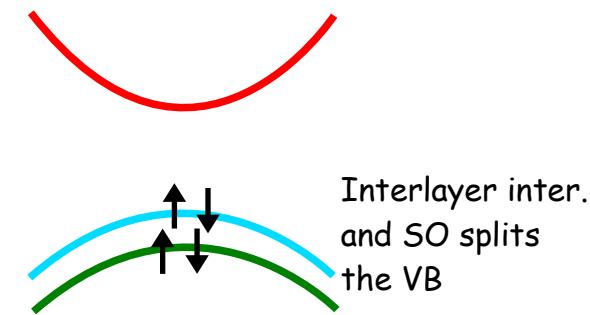
Single-layer ( $D_{3h}$ )

No inversion symmetry



Double-layer and bulk ( $D_{6h}$ )

Inversion symmetry

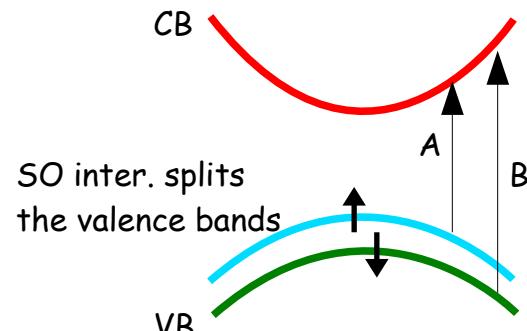


# Transition metal dichalcogenides

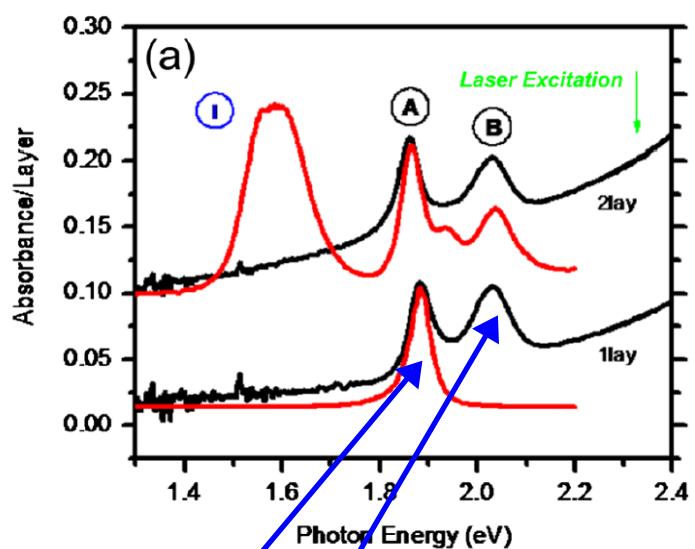
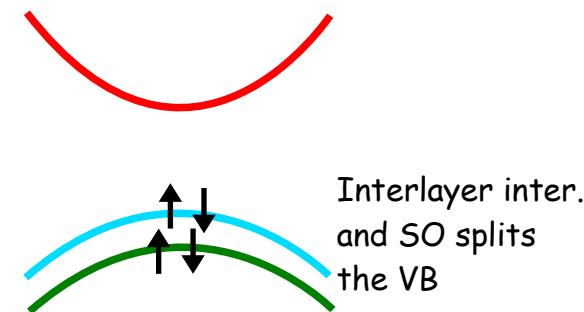
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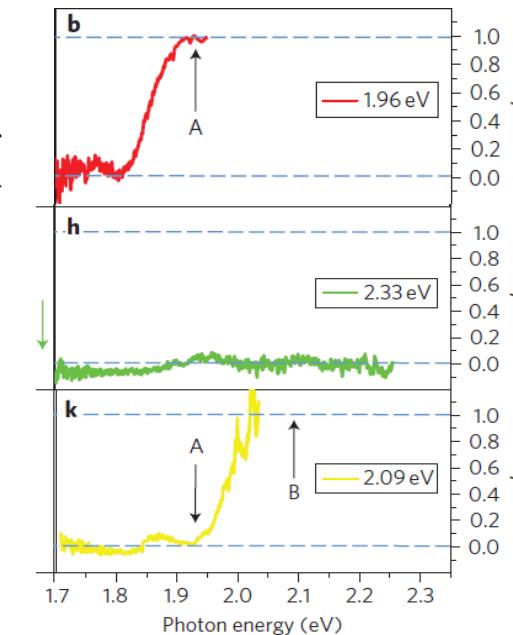
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VB splitting is exhibited in the PL and absorption by a two peaks structure



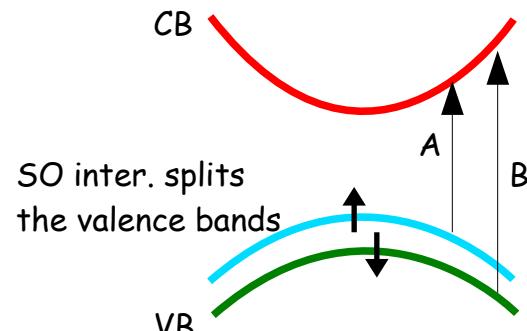
Control of the light polarization helicity by tuning the excitation energy (valley physics).

# Transition metal dichalcogenides

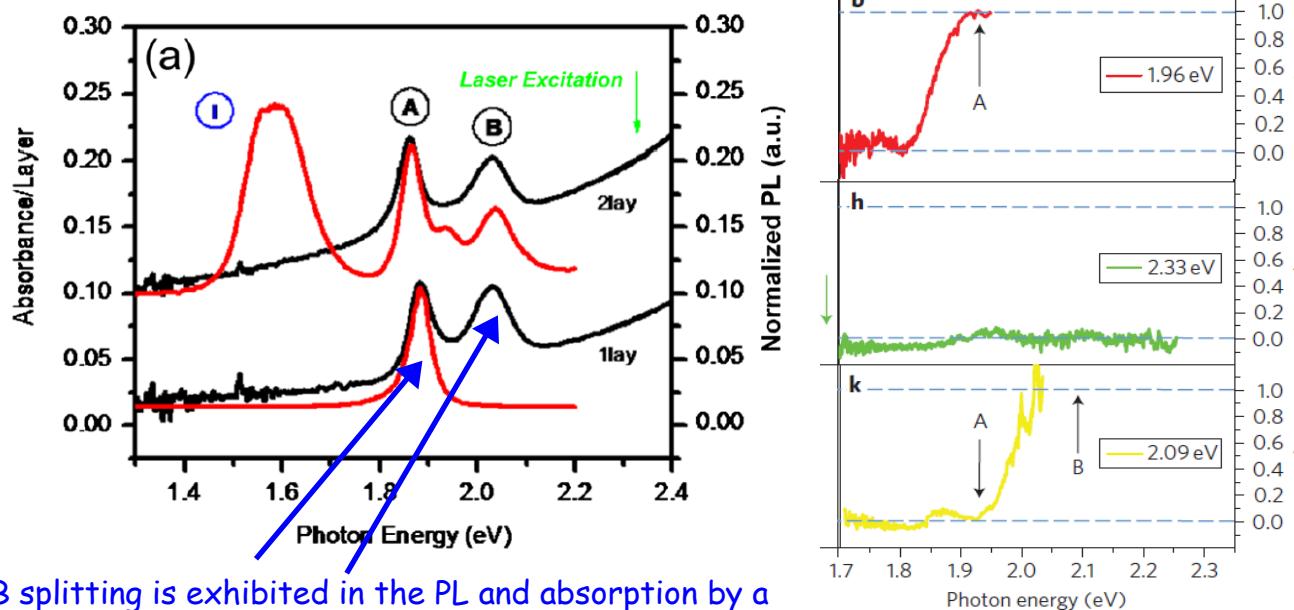
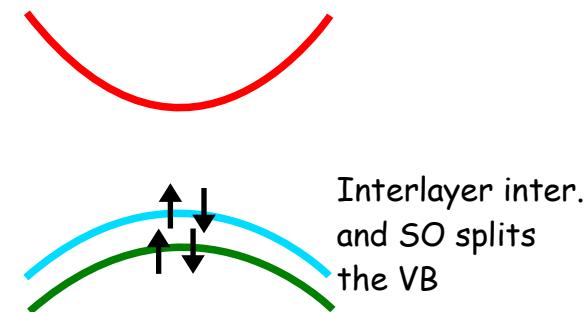
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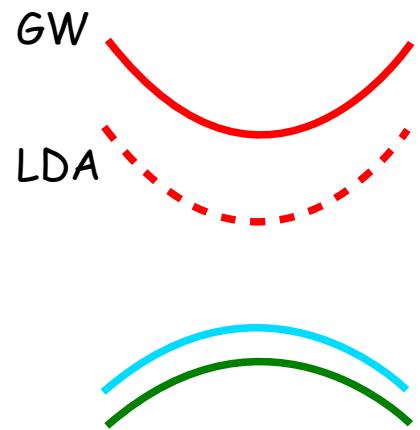


VB splitting is exhibited in the PL and absorption by a two peaks structure

Control of the light polarization helicity by tuning the excitation energy (valley physics).

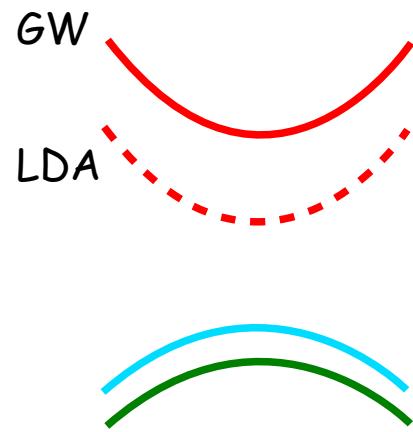
We have studied the electronic structure and the optical properties of  $\text{MoS}_2$ , and the dependence on the number of layers on the excitonic effects

# MoS<sub>2</sub>. Band Structure. LDA and GW method

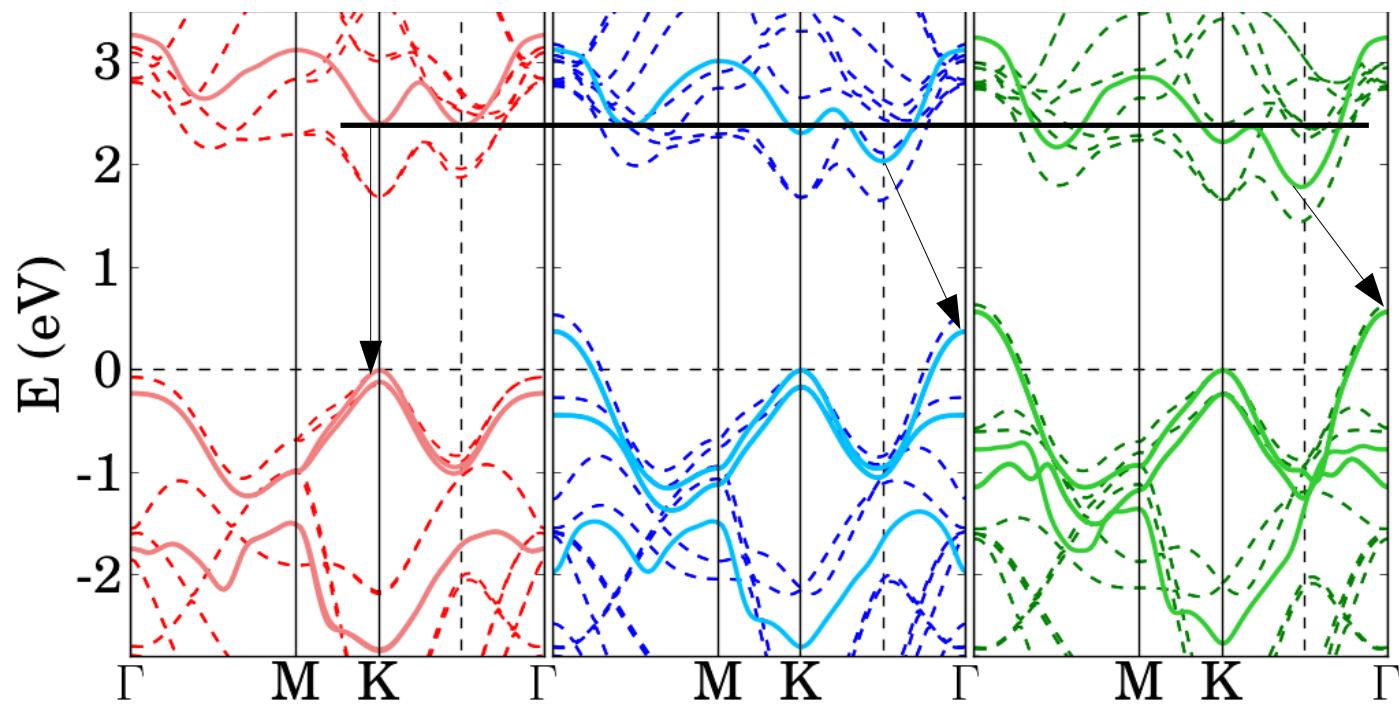


Correction of LDA bandgap  
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# MoS<sub>2</sub>. Band Structure. LDA and GW method



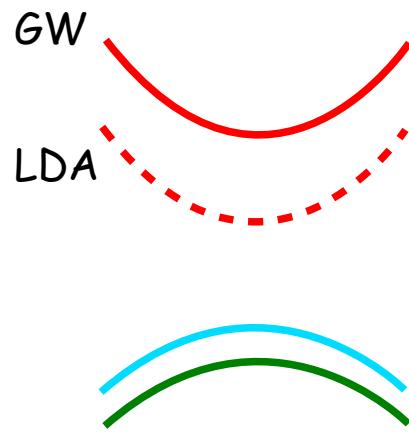
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Electronic correlation is very sensitive to variations in dielectric screening.

The addition of more layers changes the dielectric screening, the symmetry and the interlayer interaction.

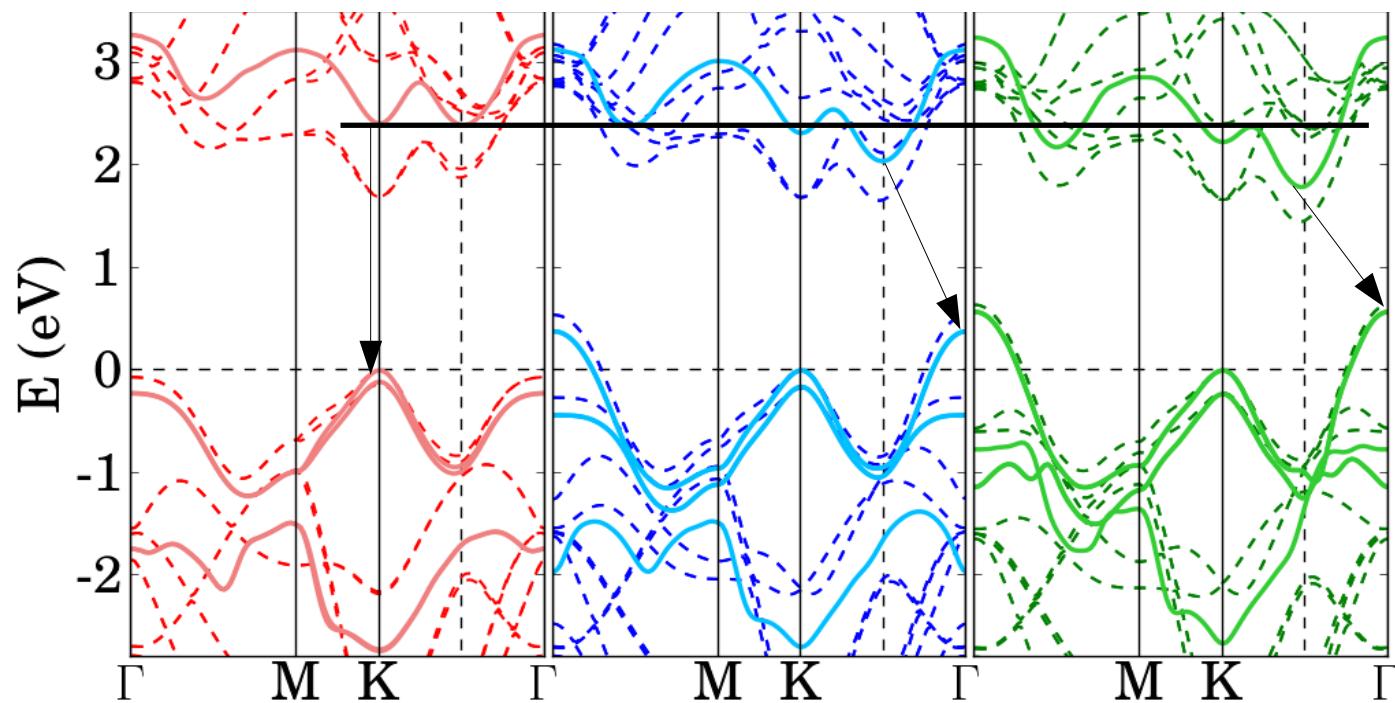
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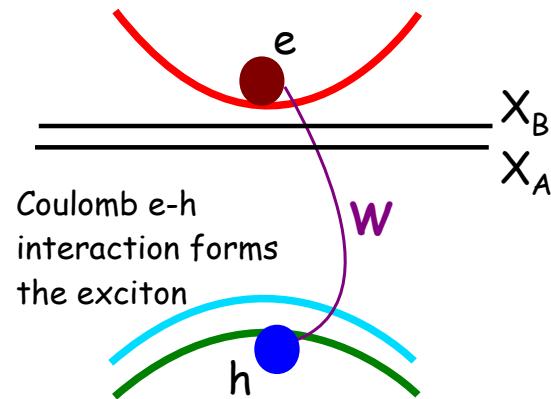


The GW correction is mainly a rigid shift of the conduction band. The correction is smaller when the number of layers increases (screening of the electron correlation).

Bandgap extremely sensitive to lattice optimization

The addition of more layers pushes up the valence band at  $\Gamma$ , making double-layer and bulk MoS<sub>2</sub> indirect SCs.  
**Excitonic effect on the optical properties...**

# MoS<sub>2</sub>. Excitonic Effects. Bethe-Salpeter Equation



$$H^{exc}_{(n_1, n_2), (n_3, n_4)} = (E_{n_2} - E_{n_1}) \delta_{(n_1, n_3)} \delta_{(n_2, n_4)} + i(f_{n_2} - f_{n_1}) \Xi_{(n_1, n_2), (n_3, n_4)}$$

Energy difference

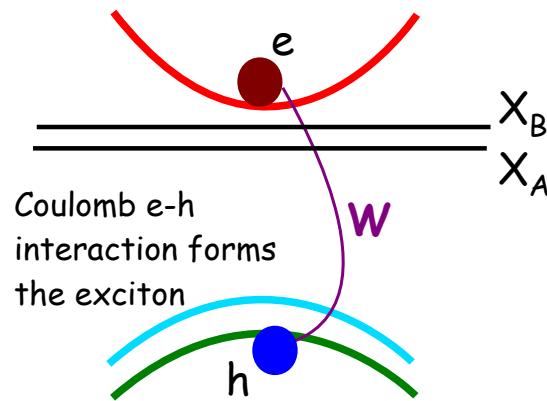
Bethe-Salpeter Kernel

$$\Xi_{\mathbf{K}_1 \mathbf{K}_2} = -iV_{\mathbf{K}_1 \mathbf{K}_2} + iW_{\mathbf{K}_1 \mathbf{K}_2} \quad \mathbf{K} \equiv (c, v, \mathbf{k})$$

Unscreened short ranged exchange interaction

Screened coulomb interaction

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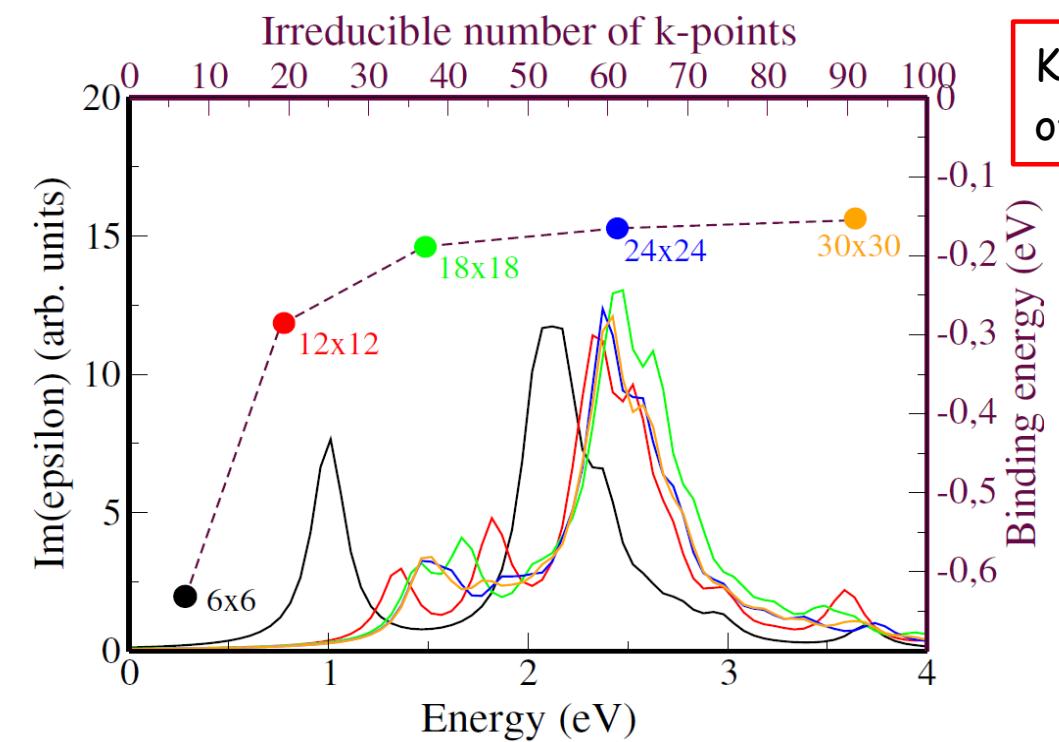
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$$+ i(f_{n_2} - f_{n_1}) \Xi_{(n_1, n_2), (n_3, n_4)}$$

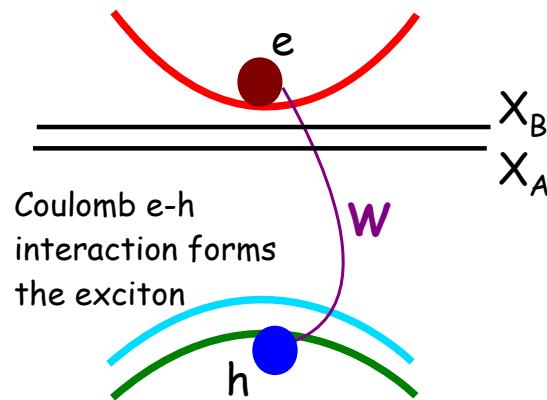
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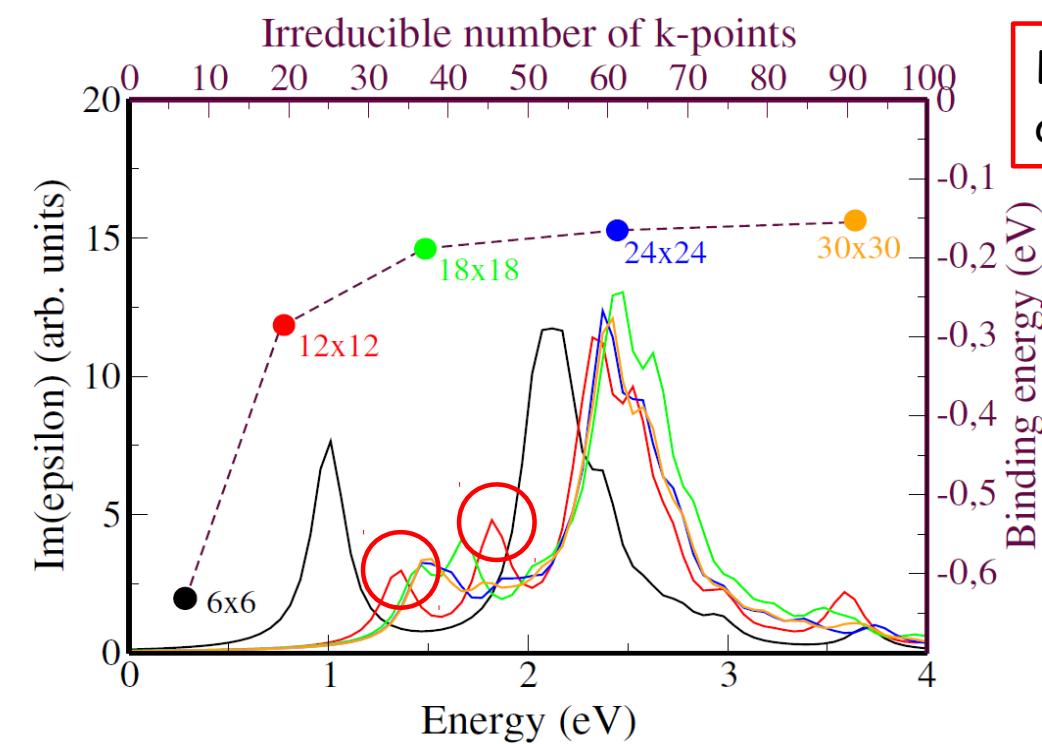
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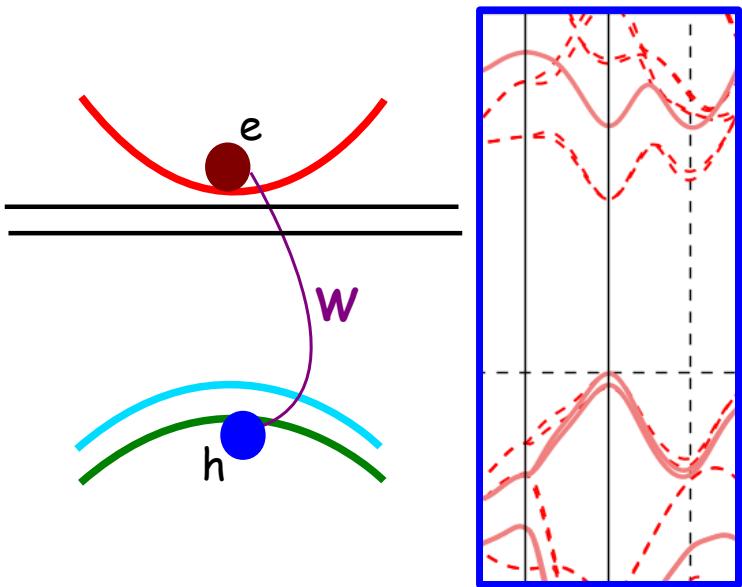
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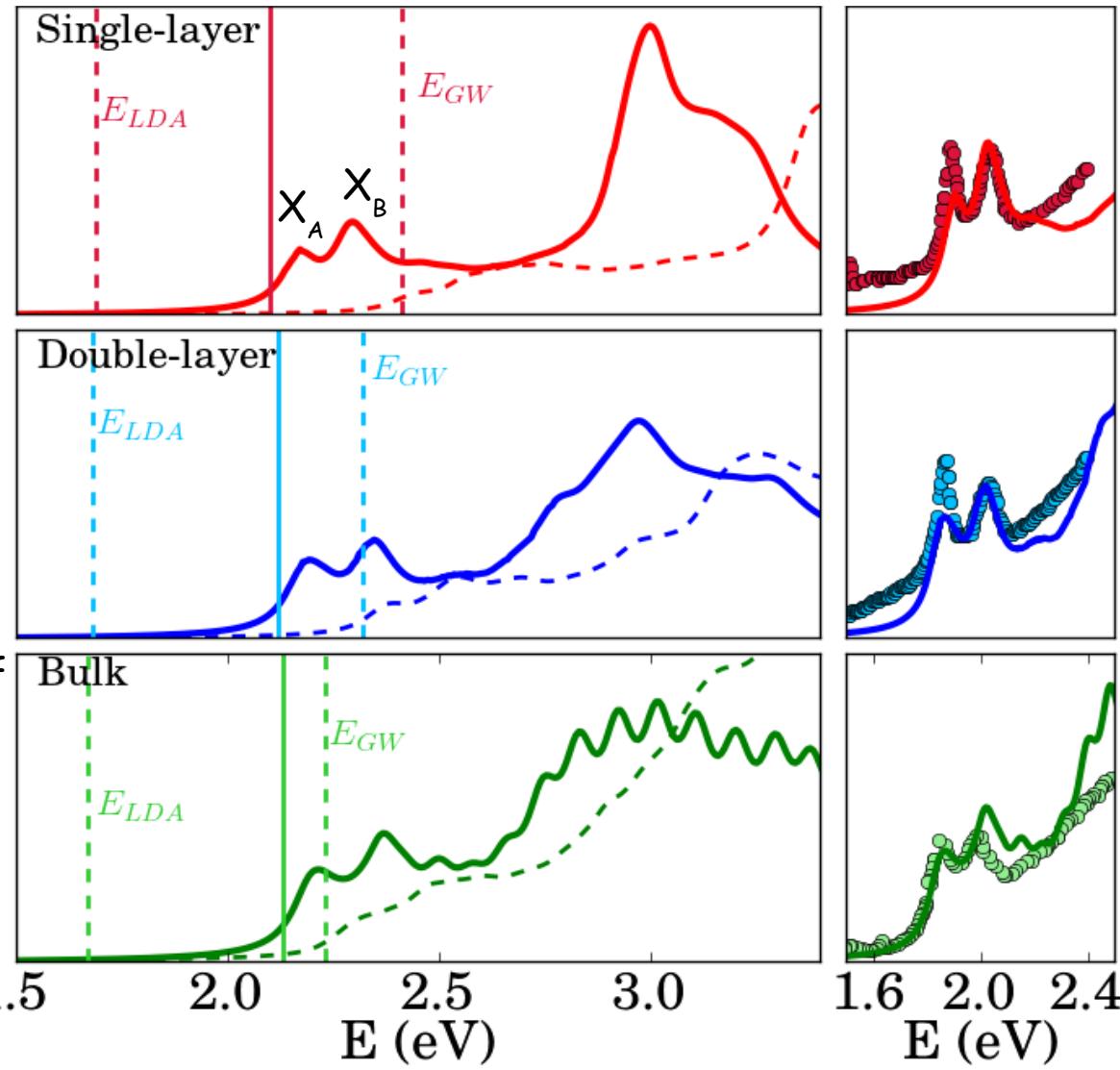
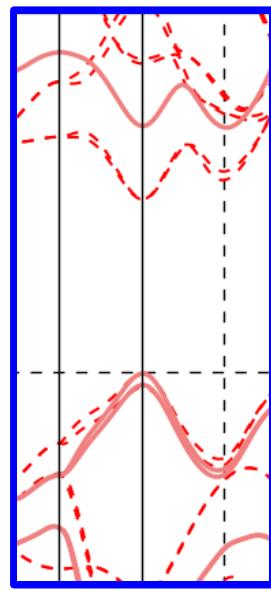
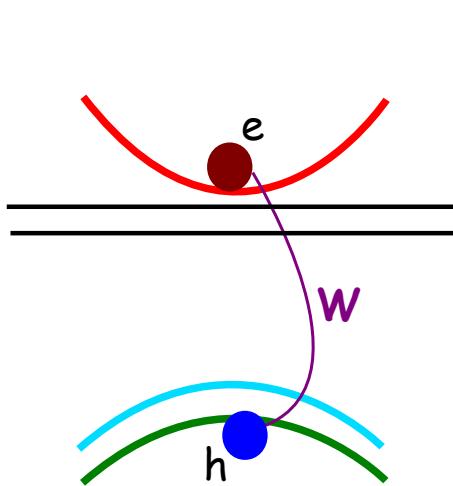
Lack of convergence in k-points normally overestimate the exciton binding energy. The k-sampling is directly related to the numbers of unit cells employed to map the exciton wave functions. Low k-sampling gives also artifacts in the optical absorption.

# MoS<sub>2</sub>. Excitonic Effects. Bethe-Salpeter Equation



The exciton binding energy decreases with the number of layers. Consequence of larger dielectric screening. This compensates partially the GW correction.

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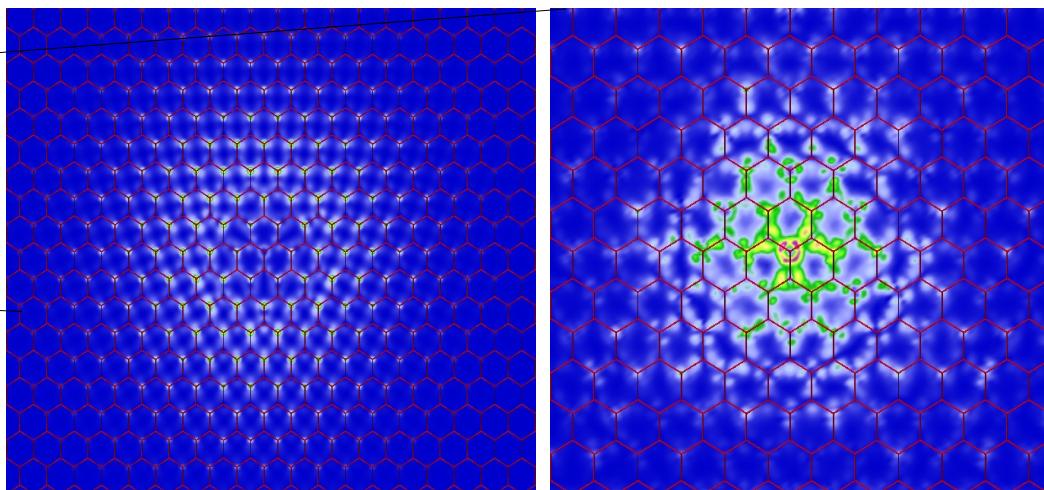
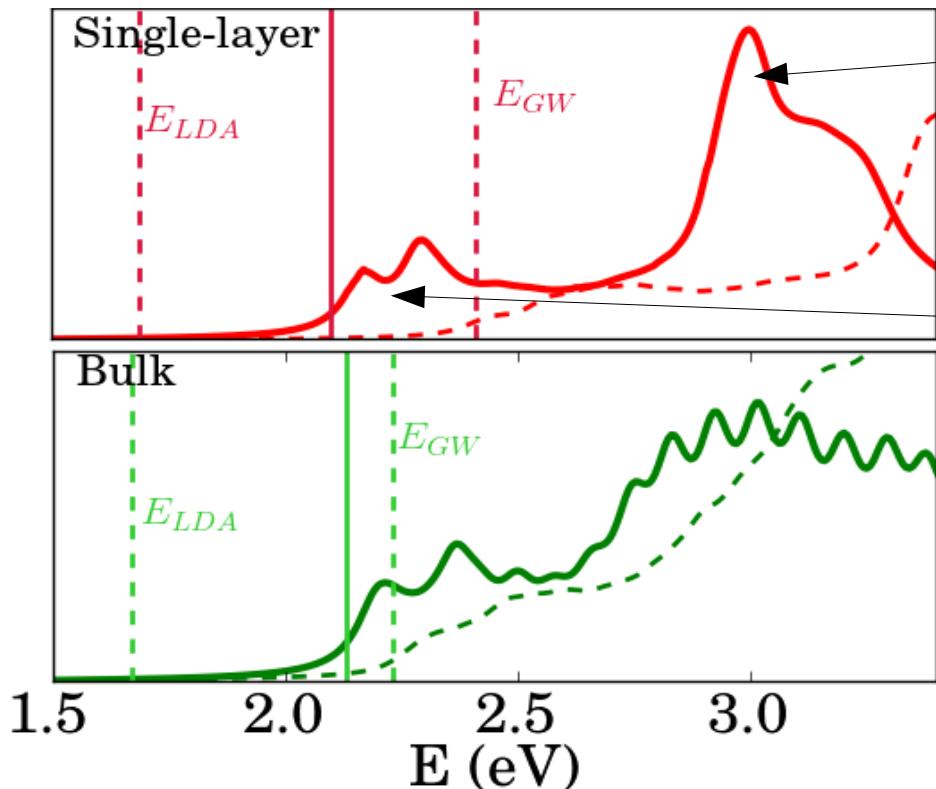


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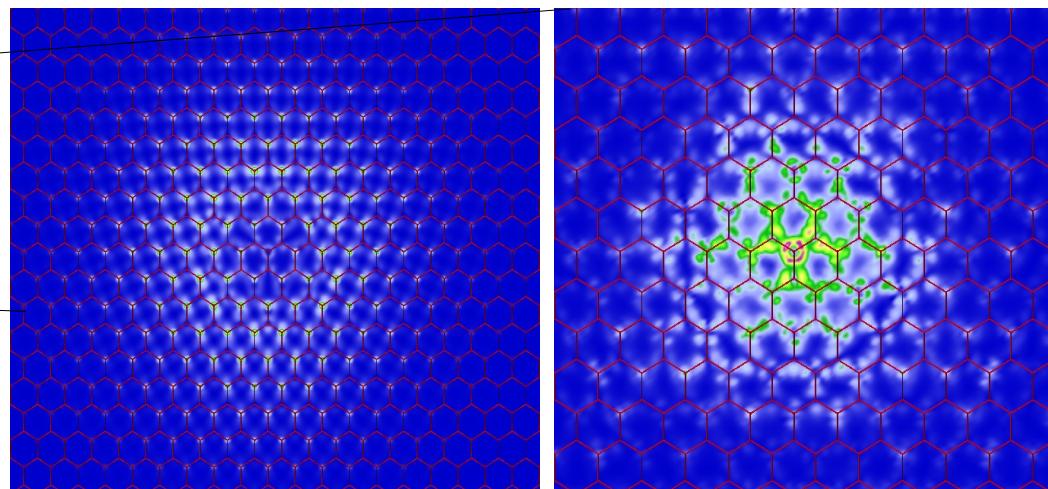
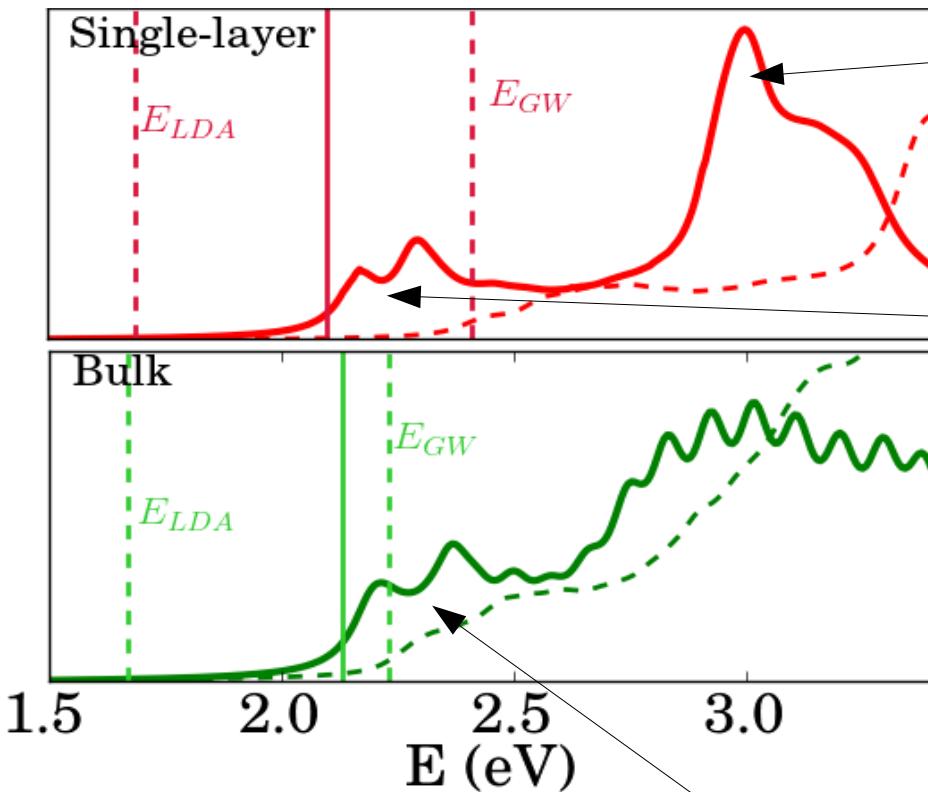
For single-layers (around 3 eV) the absorption gains in efficiency (strongly bound exciton).

The theoretical spectra captures nicely the peaks separation for all the cases.

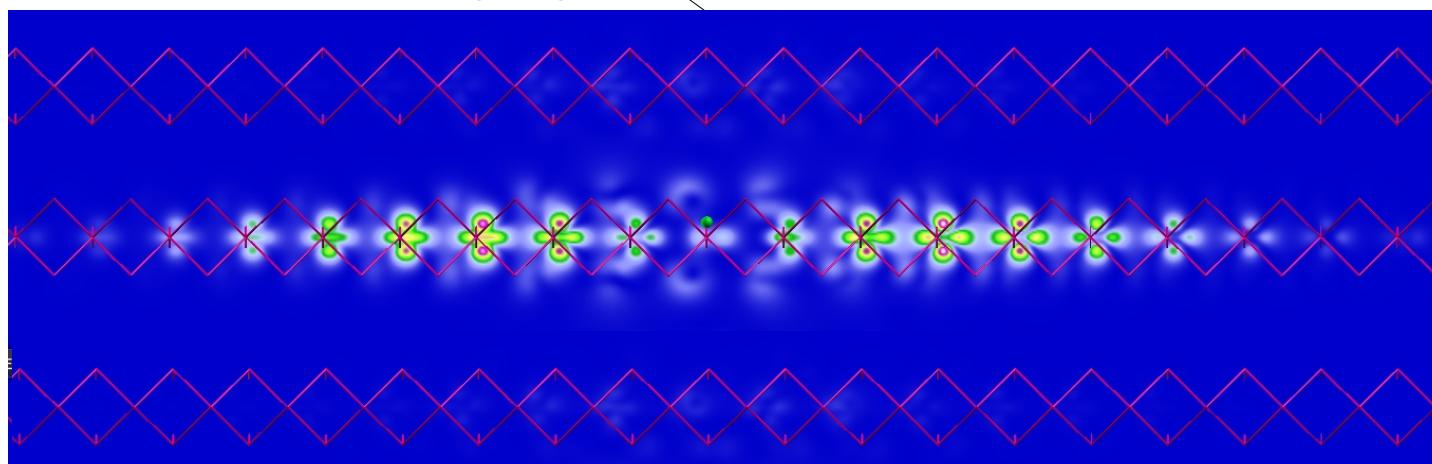
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# MoS<sub>2</sub>. Excitonic Effects. Bethe-Salpeter Equation



For bulk, the exciton is confined in only one layer, due to the large interlayer distance.



# Conclusions and ongoing work

- The bandgap (direct or indirect) depends critically on the number of layers and lattice optimization.
- Importance of convergence for reliable results.
- Excitonic effects are stronger in environments with small dielectric constant (single-layers).
- Further studies will deal with strained layers and the influence on the optical response (tunability of the bandgap).

# Acknowledgements



UNIVERSITY OF LUXEMBOURG  
Physics and Material Sciences  
Research Unit (PHYMS)

Kerstin Hummer, University of Vienna.

Davide Sangalli and Andrea Marini, Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), Rome Italy.



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Thank you for your attention!

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