# *Optical study of atomic monolayers*

CENTRO DE INVESTIGACIONES EN OPTICA, A.C.

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Seminar at CICESE

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# Introduction

## Graphene monolayer

- Novoselov, Geim et al. prepared graphitic sheets of thickness down to a few atomic layers, including a single layer graphene, to fabricate devices and to study their electronic properties. [Novoselov et al., Science, **306**, 666 (2004)]

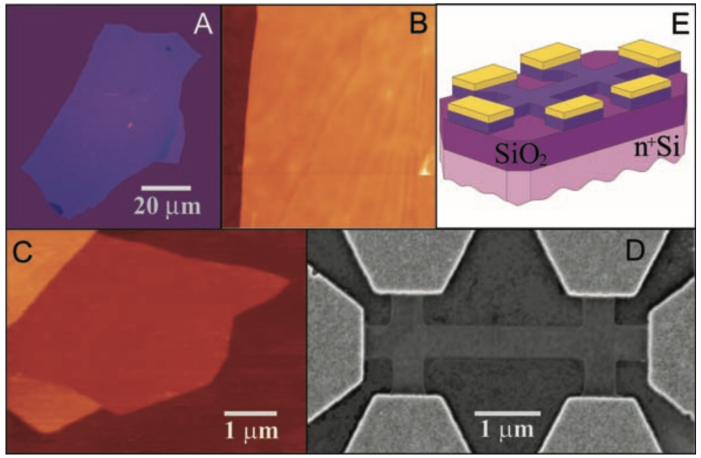


**Fig. 1.** Graphene films. (**A**) Photograph (in normal white light) of a relatively large multilayer graphene flake with thickness ~3 nm on top of an oxidized Si wafer. (**B**) Atomic force microscope (AFM) image of 2 μm by 2 μm area of this flake near its edge. Colors: dark brown, $SiO_2$ surface; orange, 3 nm height above the $SiO_2$ surface. (**C**) AFM image of single-layer graphene. Colors: dark brown, $SiO_2$ surface; brown-red (central area), 0.8 nm height; yellow-brown (bottom left), 1.2 nm; orange (top left), 2.5 nm. Notice the folded part of the film near the bottom, which exhibits a differential height of ~0.4 nm. For details of AFM imaging of single-layer graphene, see (*15*). (**D**) Scanning electron microscope image of one of our experimental devices prepared from FLG. (**E**) Schematic view of the device in (D).

# *Atomic monolayer (ML) structures*

- The discovery of the synthesis of graphene sheets stimulated the studies of other materiales arranged in atomic MLs, e.g. BN, silicene, germanene, transition metal dichalcogenade structures, phosphorene, etc.
- Two dimensional 2D structures consist of a certain number of crystalline layers.
- The physical properties of atomic ML structures differ very significantly to those of the respective bulk structures.
- Wide applications: electronic and photovoltaic devices, sensors, spintronics, etc

- Our interes focuses in the optical studies of atomic ML structures, through the calculation of their lineal, non linear and spin injection response.

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# Method

- Quantum Method - First principles
- Density Functional Theory (DFT) - LDA (GGA) Approximation
- GW method to obtain quasiparticle energies

Note: The ABINIT code has been used.

## *Steps for the calculation of the optical response*

- Calculation of the lattice constant and atomic positions.
- Calculation of the wave functions and LDA energy states.
- Calculation of the GW energies.
- Calculation of the momentum and spin matrix elements.
- Calculation of the optical response (linear, nonlinear, spin injection).

# First order optical response

## Dielectric function

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega)$$

where the imaginary part is given by:

$$\epsilon_2^{ab}(\omega) = 4\pi \Im\mathrm{m}\chi_1^{ab}(-\omega;\omega)$$

$$\epsilon_2^{ab}(\omega) = \frac{4\pi^2 e^2}{\hbar}\int \frac{\mathrm{d}\mathbf{k}}{8\pi^3}\sum_{nm} f_{nm} r^a_{nm} r^b_{mn}\delta(\omega_{mn}-\omega)$$

$\mathbf{r}_{mn}$ are the position matrix elements,
$\omega_{mn} = \omega_m - \omega_n$ are the transition frequencies between states $m$ and $n$,
$\mathbf{k}$ the wavevector,
$f_{nm} = f_n - f_m$; and the Fermi factor $f_n = (1, 0)$, for (valence, conduction) bands.
[J.E. Sipe and A.I. Shkrebtii, PRB **61**, 5337 (2000)]

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# *Layered* $In_2Se_3$ structures

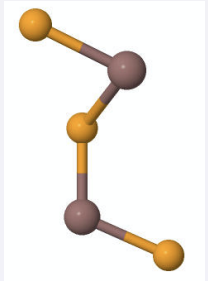
- Indium Selenide $In_2Se_3$ layered structures have attracted attention.
- Due to its polymorphism, $In_2Se_3$ have different phases $\alpha$, $\beta$, $\gamma$.
- The $\alpha$ phase has the lowest energy and belongs to the R3m space group.
- The layered estructure consists of 5 atomic layers
- Ding et al. demostrated the ferroelectric nature of $In_2Se_3$ QL [Ding et al., Nature Comm. **8**, 14956 (2017)].
- Zhou et al. reported the first experimental evidence of the out-of-plane ferroelectricity for the layered $\alpha$-$In_2Se_3$ structure. [Y. Zhou et al. Nano Letters, **17**, 5508 (2017)]
- Ding et al. theoretically found two possible stable atomic configurations within 1QL: the wurtzite and zincblende type denoted by FE-ZB' and FE-WZ'.
- Applications: memory devices, thin films ferroelectrics, sensors, etc.

# $\alpha$-$In_2Se_3$ structures

FE-ZB' - 1QL

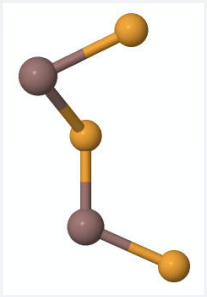
Unit cell

a=4.106 Å

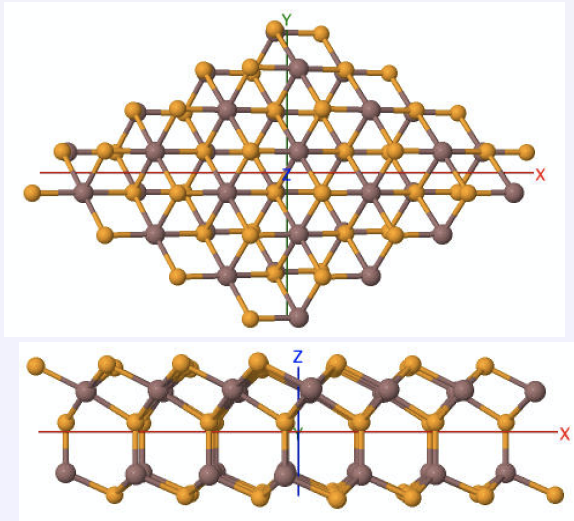


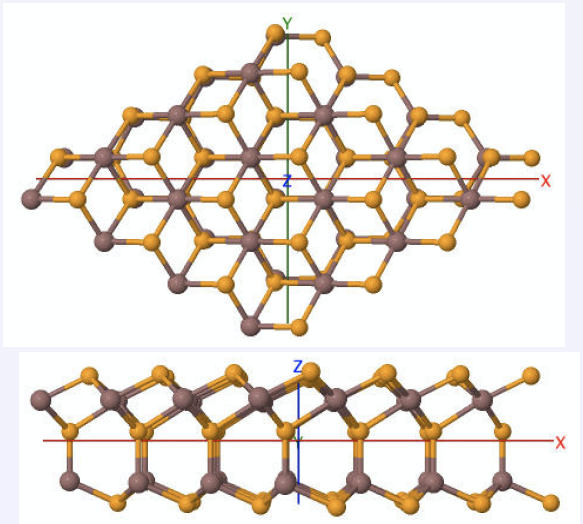
FE-WZ' - 1QL

a=4.106 Å

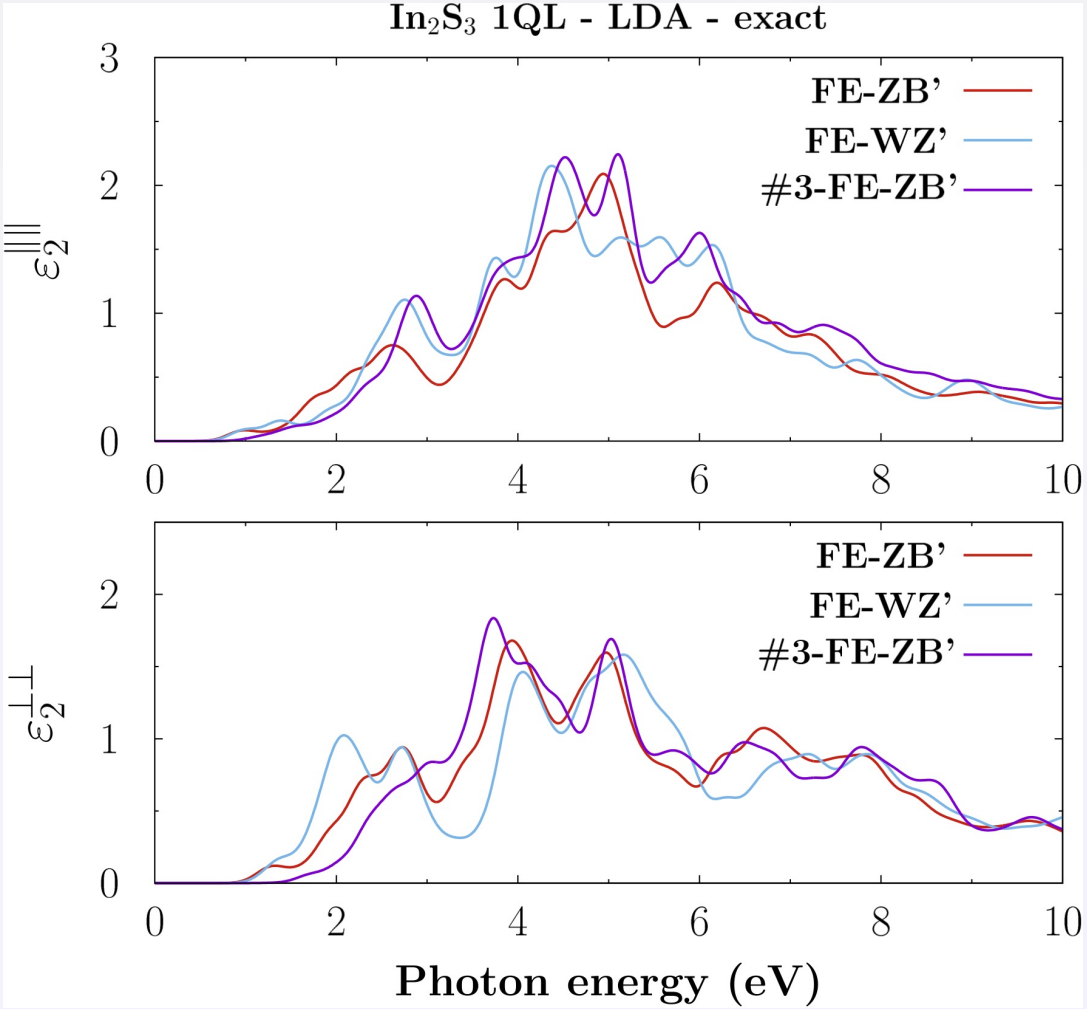


Top and side views



# *Dielectric function* $\varepsilon_2(\hbar\omega)$




Parameter values:

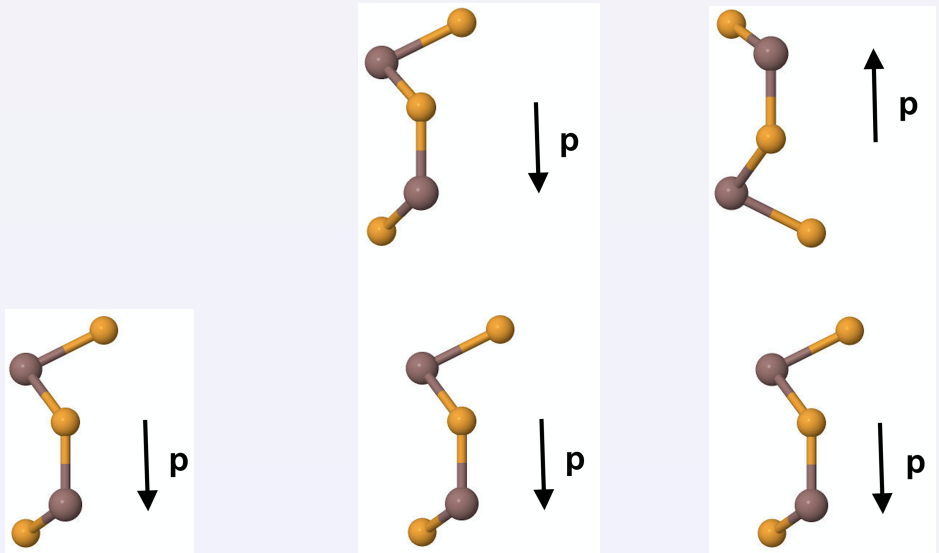
psp: HGH;
$E_c$ =40 Ha
nkpt=324 (IBZ)
Vaccuum lenght = 2c
$E_g^{LDA}$=0.62 eV
$E_g^{exp}$=1.3 eV

[Jacobs-Gedrim et al. ACS Nano, **8, 514 (2014)**]

#3-FE-ZB' curve correspond to FE-ZB' structure with $a$ =3.987 Å

# *Ferroelectric nature of* $In_2Se_3$

Ding et al. demostrated the ferroelectric nature of $In_2Se_3$ QL as a result of the lost of centrosymmetry of the middle Se atom. It presents both out-of-plane and in-plane electric polarization. [Ding et al., Nature Comm. **8**, 14956 (2017)].




(a) (b) (c)

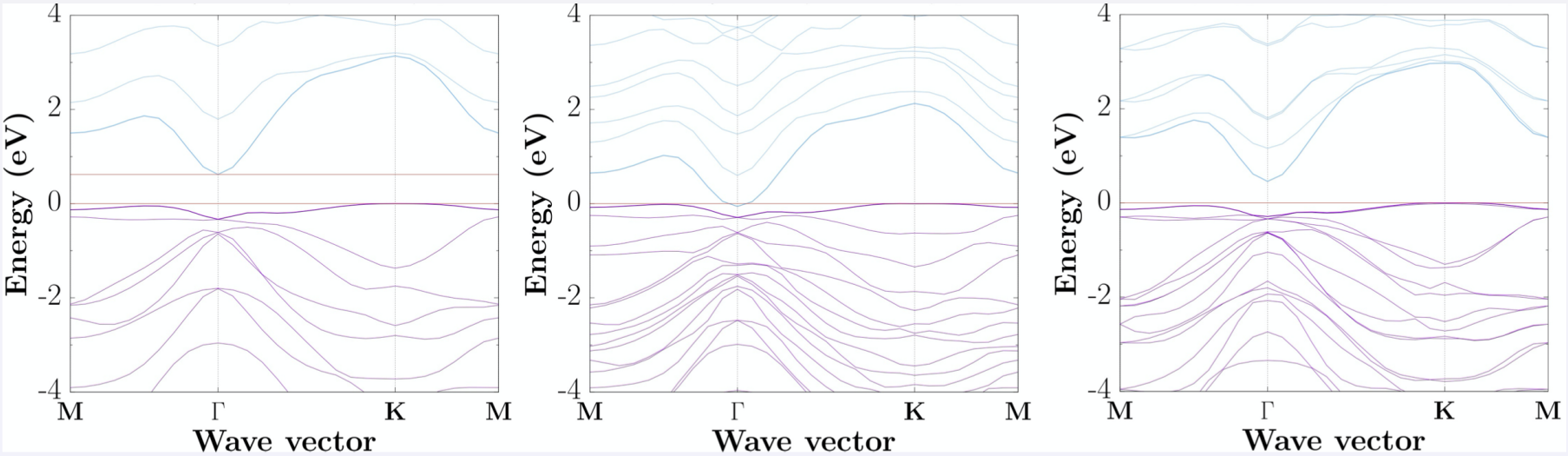
Unit cells of the $In_2Se_3$ FE-WZ' structures: for 1QL (a) and for 2QLs with a net non-zero (b) and zero (c) electric dipole moments.

# *Band structures for $In_2Se_3$ FE-WZ'*

FE-WZ' - 1QL

FE-WZ' - 2QL
net $\vec{p}$

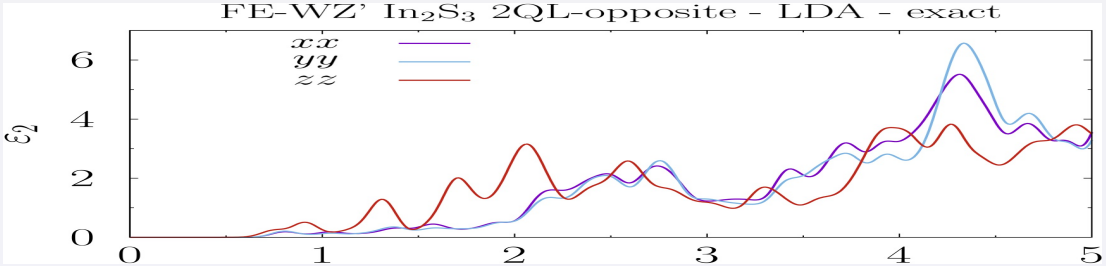
FE-WZ' - 2QL
opposite $\vec{p} = 0$



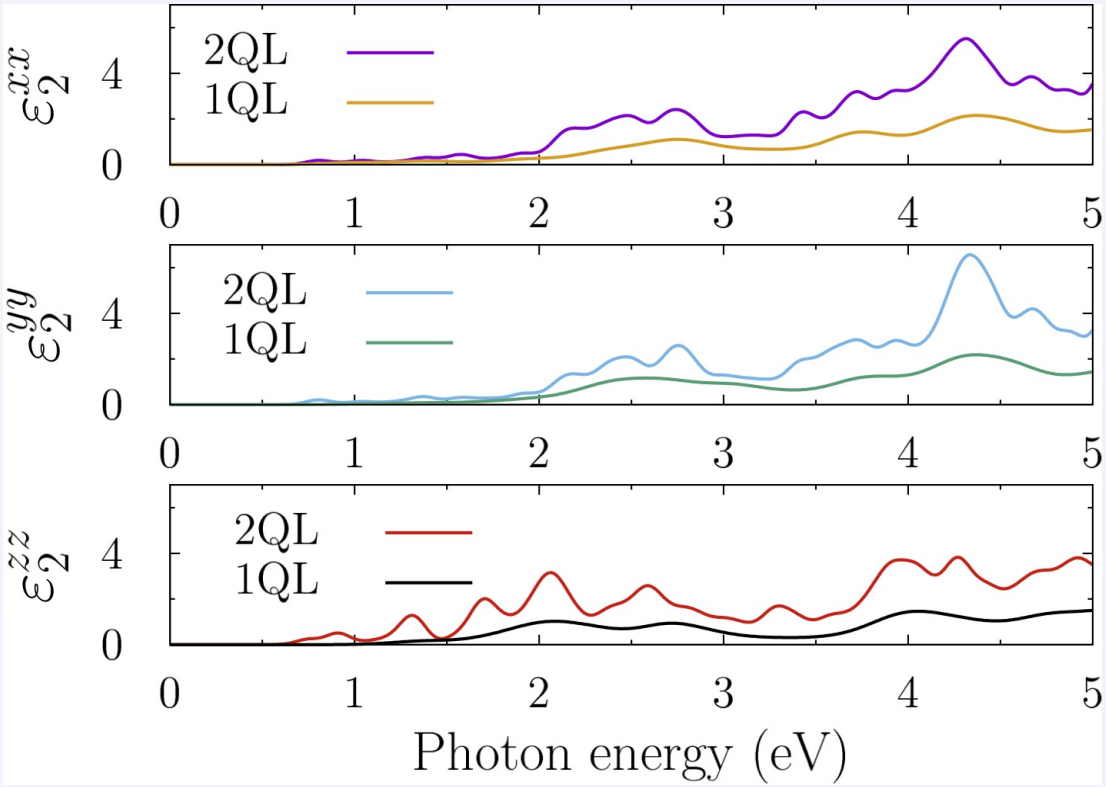

Parameter values: psp: HGH; $E_c$ =40 Ha Vaccuum lenght = 2c
For 1 ML: $E_g^{LDA}$ =0.62 eV; $E_g^{LDA-sc}$ =0.58 eV; $E_g^{GGA}$ =0.79 eV (Ding);
$E_g^{exp}$ =1.3 eV [ACS Nano, **8**, 514 (2014)];
For 2ML (net $\vec{p}$): There is no band gap in LDA;
For 2ML ($\vec{p} = 0$): $E_g^{LDA}$ =0.46 eV. (indirect); $E_g^{LDA}$ =0.75 eV. (direct);

# *Dielectric function* $\varepsilon_2(\hbar\omega)$

## FE-WZ' 2QL structure with $\vec{p} = 0$




## Comparison: 2QL $\vec{p} = 0$ Vs 1QL




Parameter values:

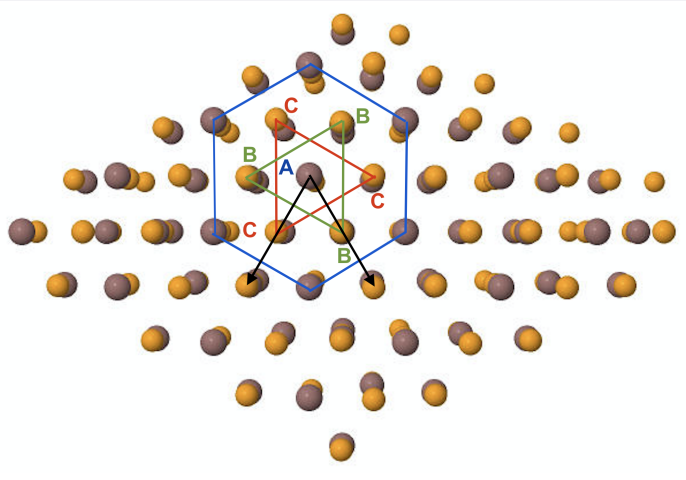
psp: HGH;
$E_c$ =40 Ha
nkpt=324 (IBZ)
Vaccuum lenght = 2c

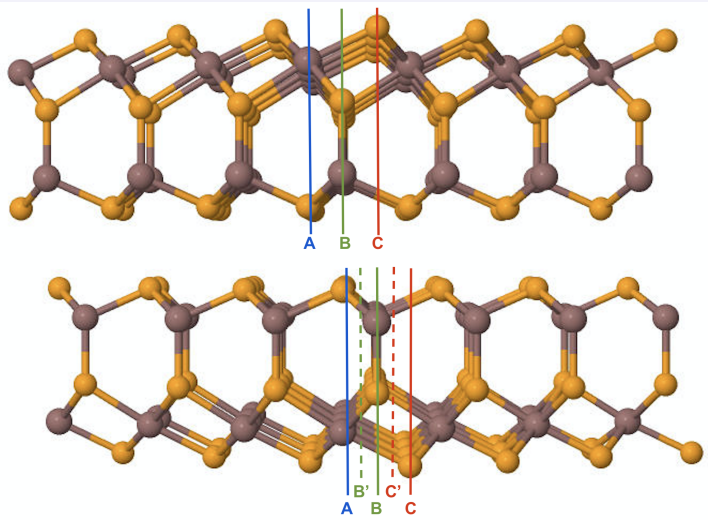
For 1 ML:
$E_g^{LDA}$ =0.62 eV;
$E_g^{exp}$ =1.3 eV [ACS Nano, **8**, 514 (2014)];

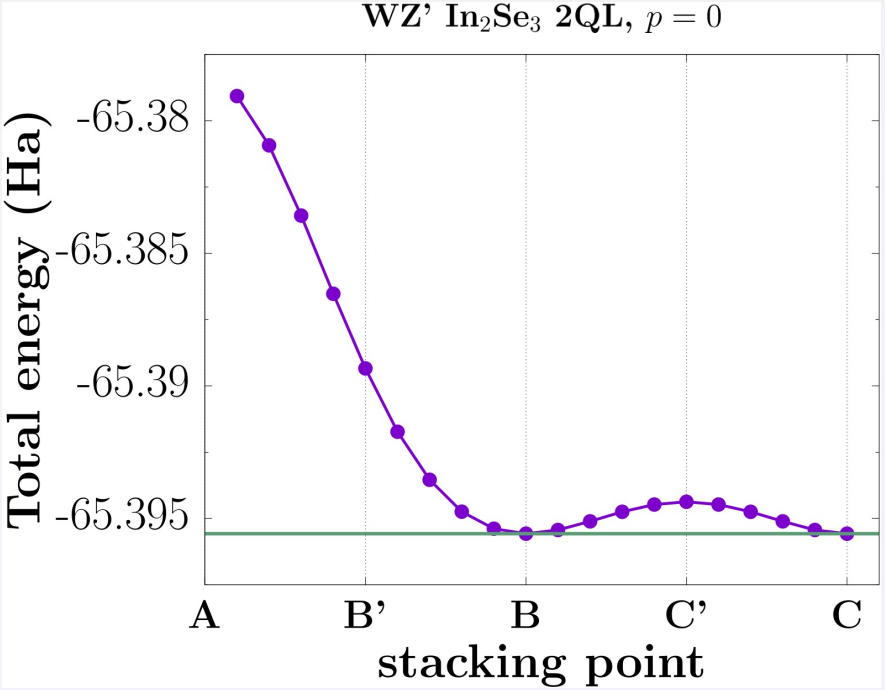
For 2ML ($\vec{p} = 0$):
$E_g^{LDA}$ =0.46 eV. (I);
$E_g^{LDA}$ =0.75 eV. (D);

# *Total energy Vs stacking point*

FE-WZ' - $In_2Se_3$ 2QL, $\vec{p} = 0$



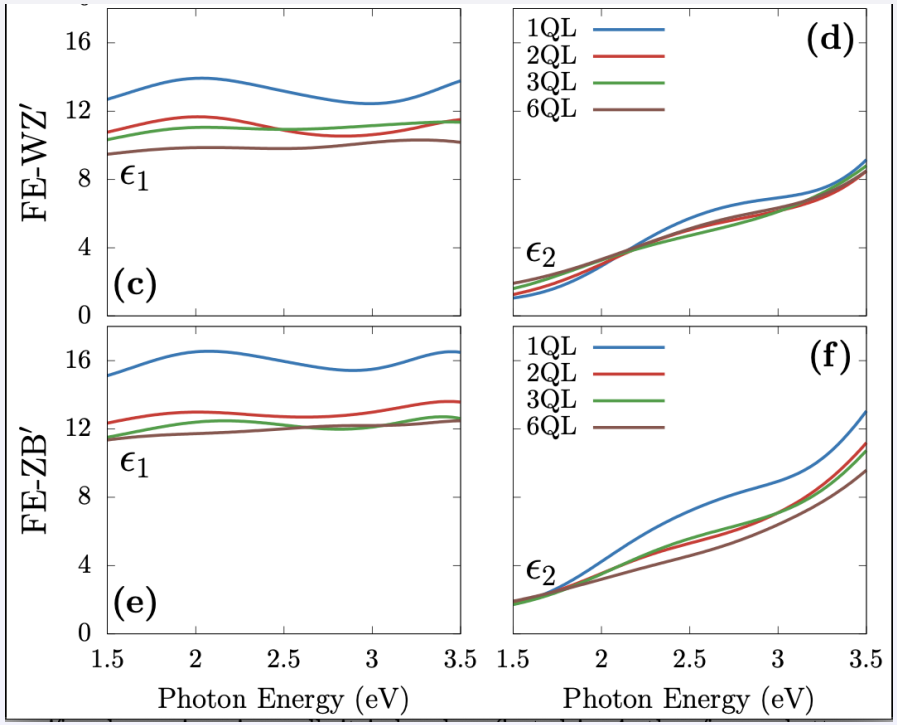

The unit cell of the bulk is repeated every 3QLs

Type of stacking: AAA, ABC, ACB, etc.

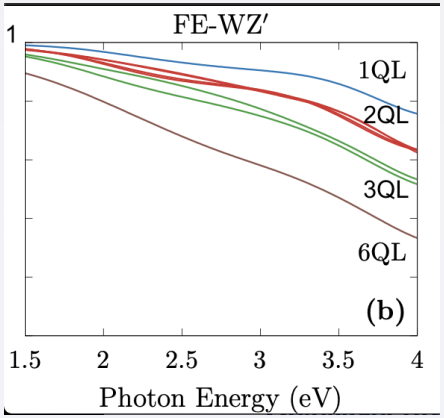
# *Dielectric function and Transmission*

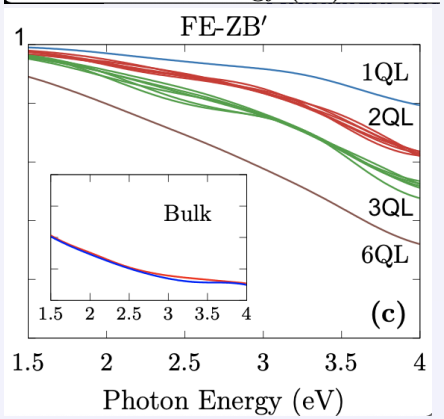
For the $\alpha$-$In_2Se_3$ structure.

Dielectric function




Transmission

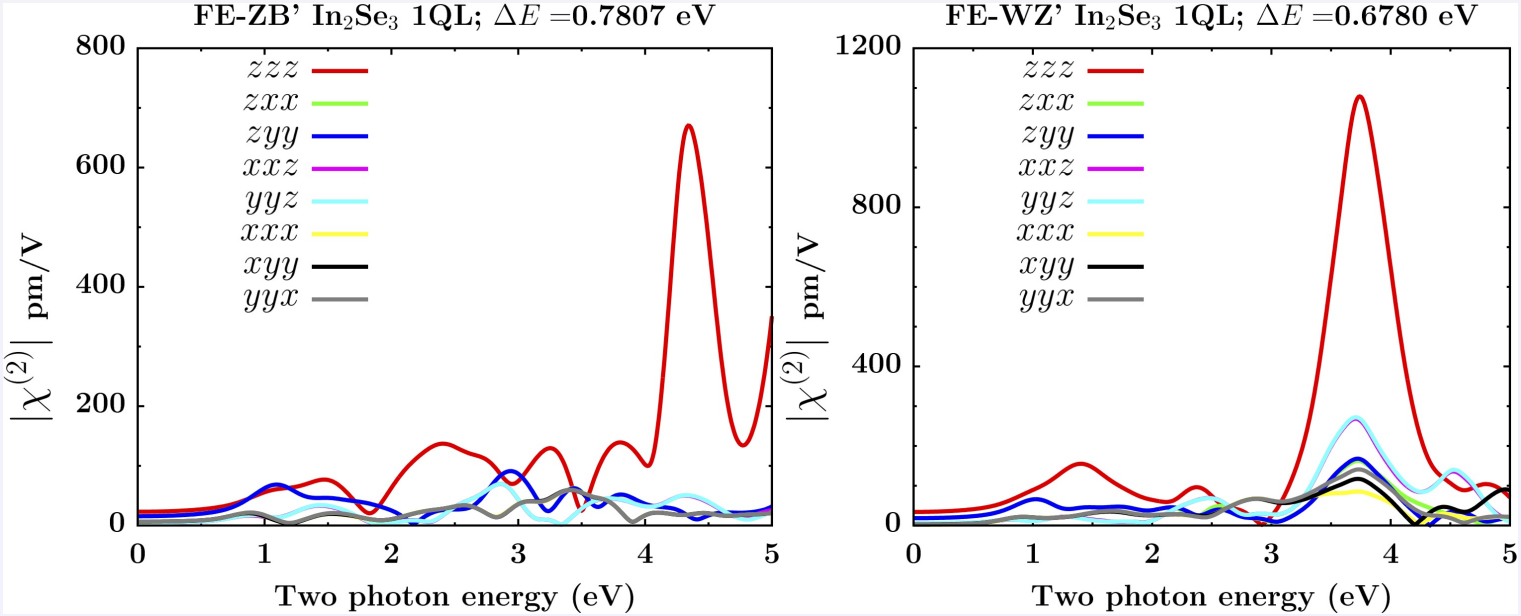



- Different dielectric function curves are generated by averaging over the various stacking arrangements.
- Different transmission curves with the same color correspond to the various stacking arrangements.

# *Second order response* $|\chi^{(2)}|$

- $\alpha$-$In_2Se_3$ structure belongs to the R3m symmetry group and has four independent non-vanishing components of the NL susceptibility: $zzz$, $zxx = zyy$, $xxz = yyz$, $xxx = xyy = yyx$




- The second order NL susceptibility is sensitive to changes to the atomic structure.

## Summary

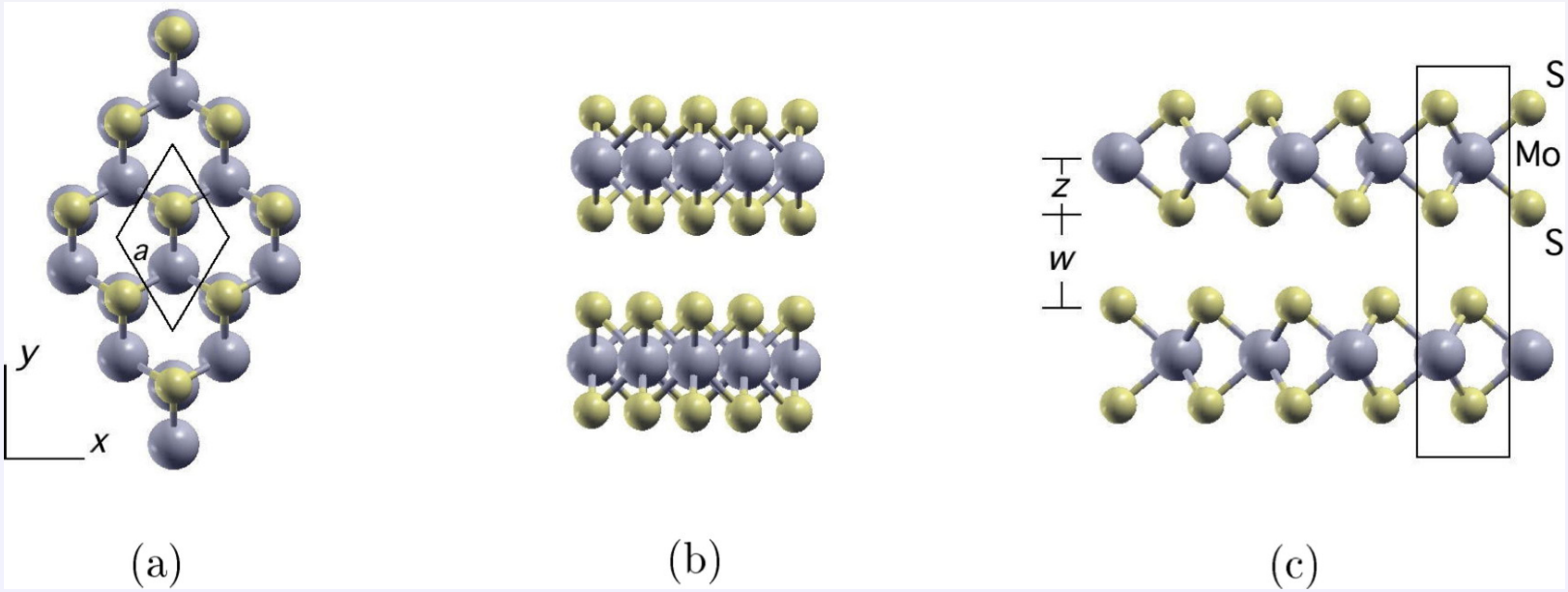
- We have studied the linear and non linear optical response of $\alpha$-$In_2Se_3$ structure

## Conclusions

- The linear response is sensitive to the number of QLs or thicknesses of the structure.
- The transmission spectra in overall decrese as the number of QLs increase.
- The nonlinear optical response is more sensitive to changes in the atomic structure.

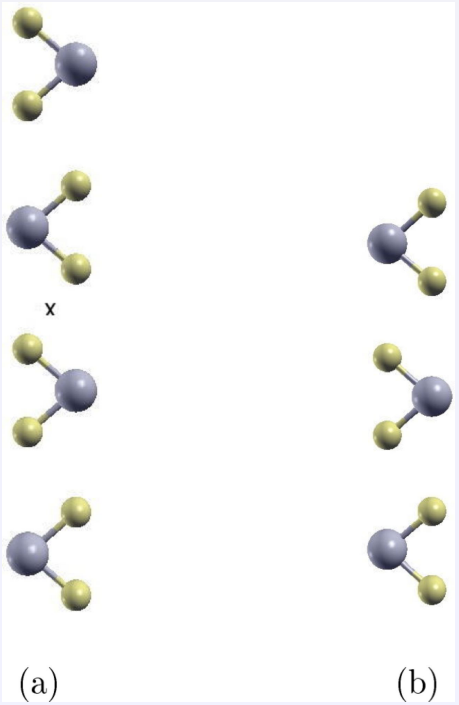
# $MoS_2$ monolayer structure

ATOMIC STRUCTURE: 2H-$MoS_2$, hexagonal, ABAB stacking
FAMILY: Transition-metal dichalcogenides
SPATIAL GROUP FOR THE BULK STRUCTURE: $P6_3/mmc$
SPATIAL GROUP FOR THE MONOLAYER STRUCTURE: $P\bar{6}m2$

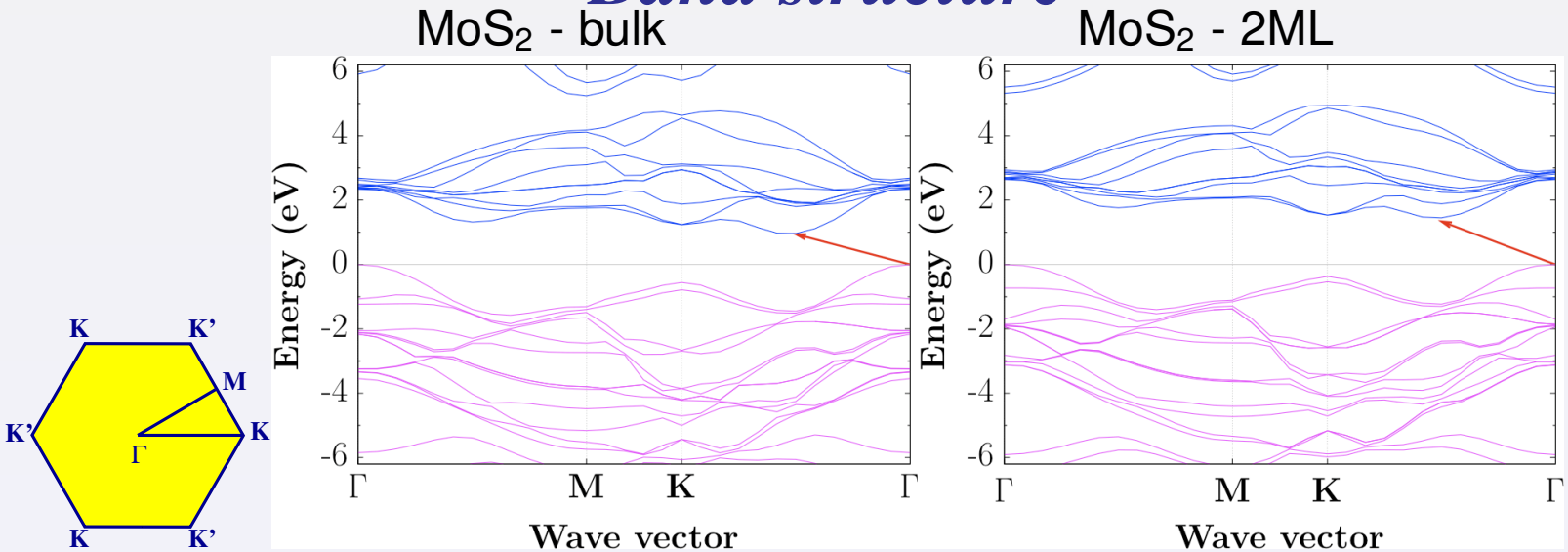


# *Characteristics of the $MoS_2$ structures*

- The bulk structure of $MoS_2$ is centrosymmetric (CS).
- Monolayer structures of $MoS_2$ with an even number of layers are CS.
- Monolayer structures of $MoS_2$ with an odd number of layers are non CS.



# Band structure

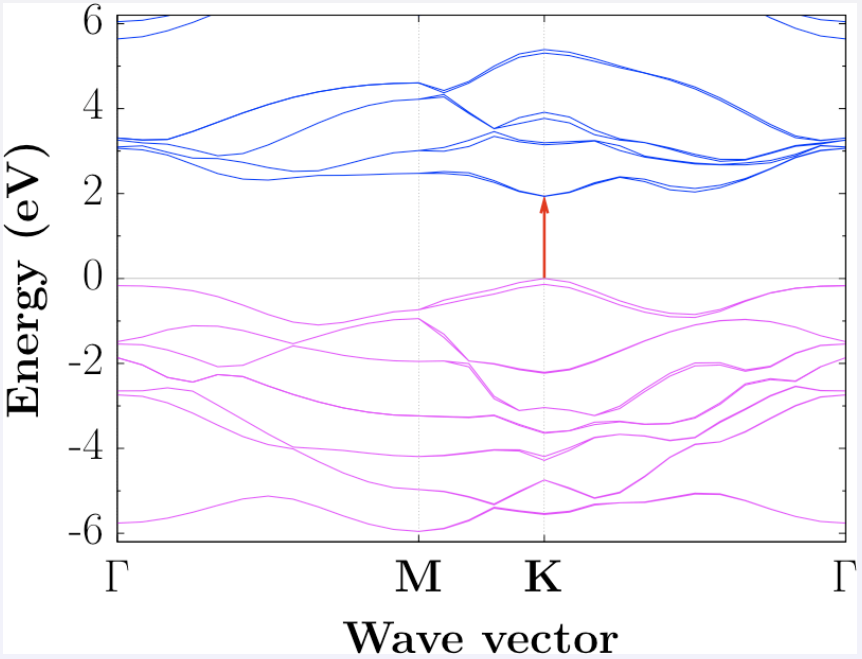


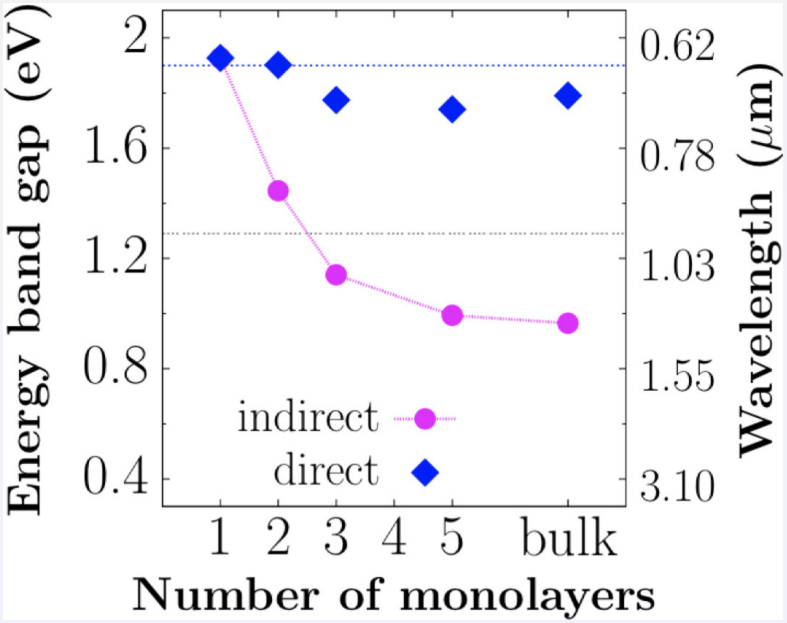

## Calculus

- Lattice constant (exp): $a = 3.16$ Å, $c = 12.296$ Å.
- Calculus of the wave functions and eigenenergies using DFT-LDA with the help of abinit.
- Relativistic pseudopotentials (HGH).
  *v e* (*s* and *p*) for S; and 6 *v e* (*s* and *d*) for Mo.
- GW Correction of the LDA band gap energy at Γ.
- The ML structure was modeled as a supercell.

# *Band structure of $MoS_2$-ML*

$MoS_2$ - 1ML



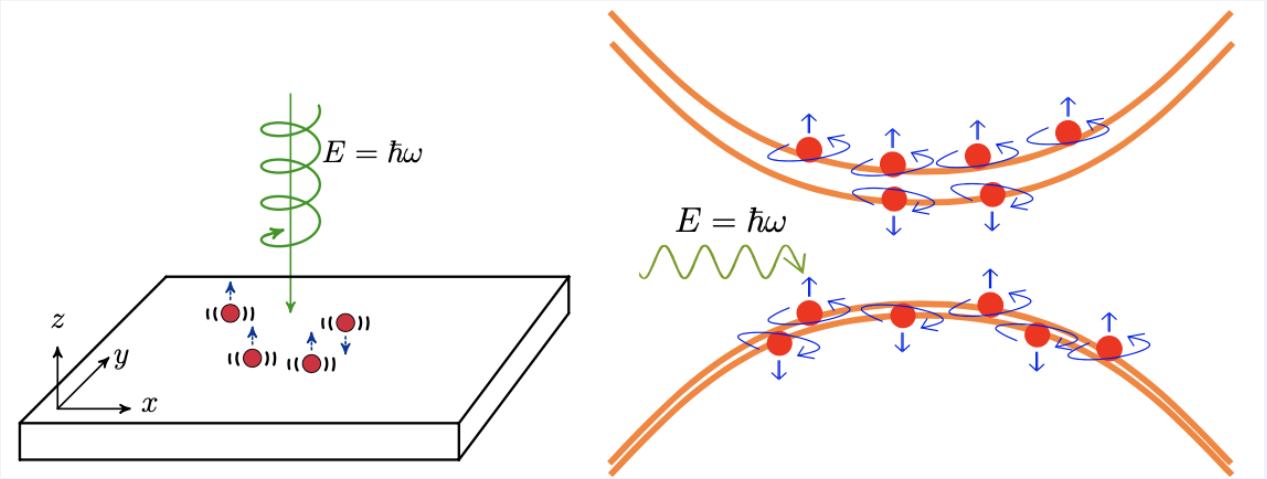




| $MoS_2$ structure | *Splitting* (meV) | $\Delta E_g$ (eV) | $E_g$ (eV) Theory I | Theory D | Experiment[1] I | Experiment[1] D |
|---|---|---|---|---|---|---|
| bulk | 231 | 0.11 | 0.97 | 1.79 | 1.29 | 1.88 |
| 2 ml | 166 | 0.19 | 1.45 | 1.90 | 1.59 | 1.88 |
| 1 ml | 137 | 0.21 | | 1.93 | | 1.90 |

[1] A.R. Beal and H.P. Hughes, J. Phys. C **12** 881 (1979),
K.F. Mak et al. Phys. Rev. Lett. **105**, 136805 (2010).

# *Spin injection in semiconductors*

- Spin-polarized electrons can be generated in the conduction bands of nonmagnetic semiconductors $\tau_e$ (ps-ns)$>>$ $\tau_h$ (fs).
  - Electrical injection. J. Phys. Condens. Matter, **28** 453003 (2016)
  - Optical injection: by one or two-photon absorption of circularly polarized light.
    PRB, **71**, 035209 (2005), PRL **90**, 216601 (2003).

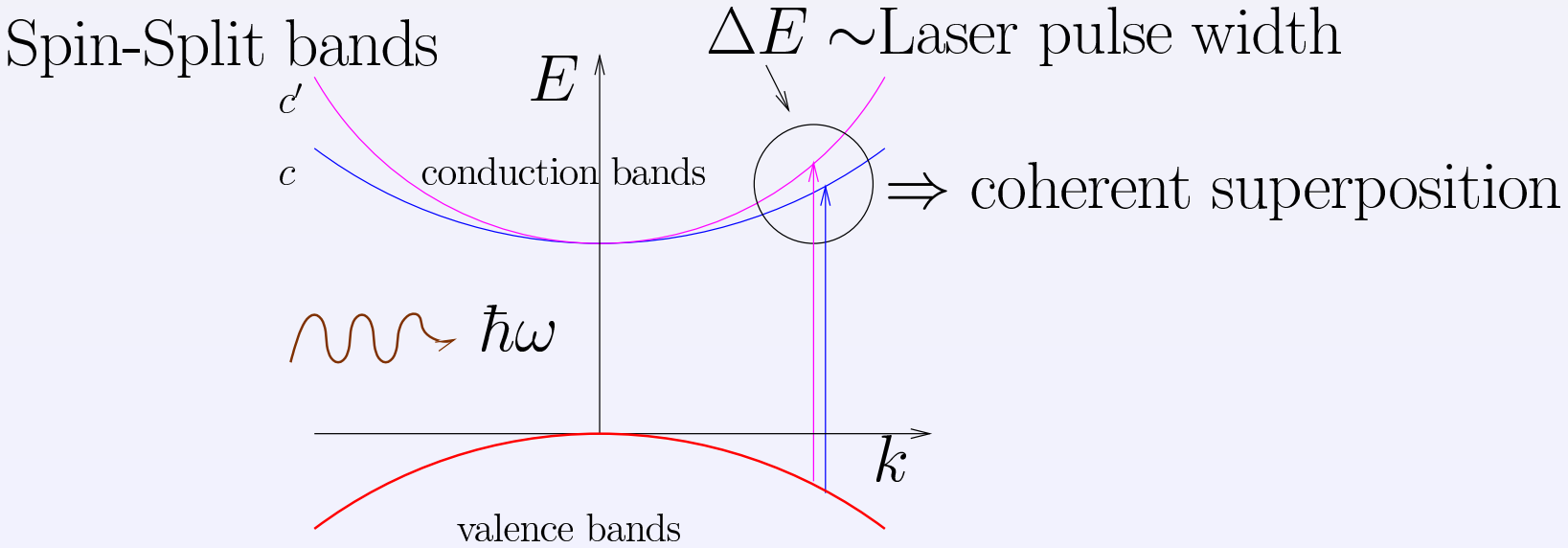


# *Optical spin injection*

The optical spin generation is based on:

- The absorption of circularly polarized light.
- Optical selection rules.
- The spin-orbit (SO) interaction.

In the process of spin injection, there is an interference between two coherent spin states, whose energy difference is $\Delta E \approx$ meV

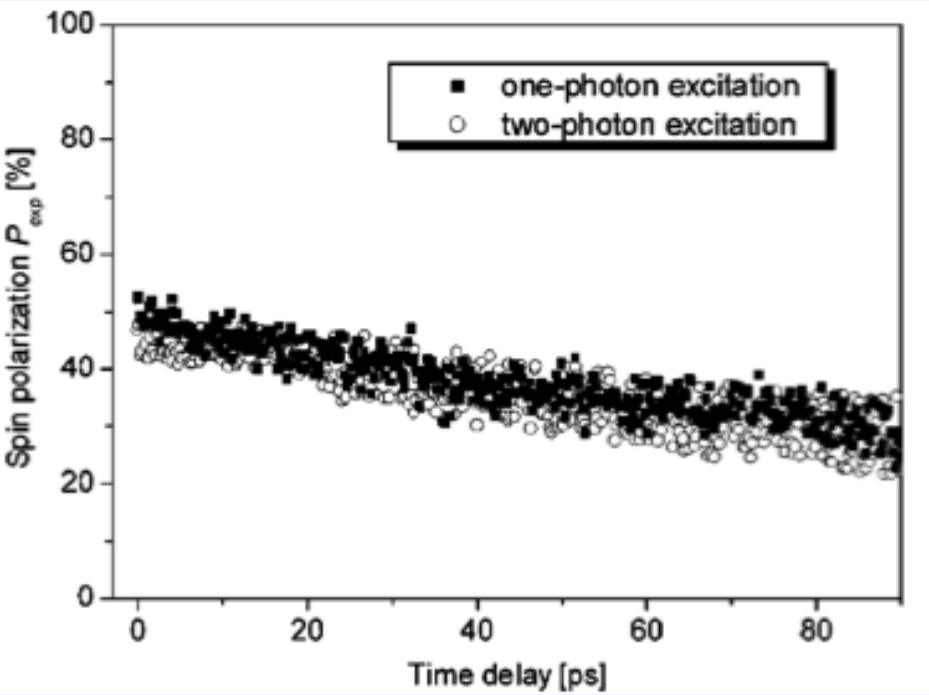


# *Degree of spin polarization* (DSP)

$$\mathrm{DSP} = \frac{N_{\downarrow} - N_{\uparrow}}{N_{\downarrow} + N_{\uparrow}}$$

$N_{\downarrow}$ ($N_{\uparrow}$) is the density of spin-down (-up) polarized electrons.

Experiment: Polarization resolved pump probe experiment in GaAs.




Bhat et al., PRB, **71**, 035209 (2005)

- Bath et al. calculated DSP as a function of excess energy for GaAs, InP, GaSb, InSb, y ZnSe.
- These materials present 50% of DSP just at the band gap energy for one-photon excitation.

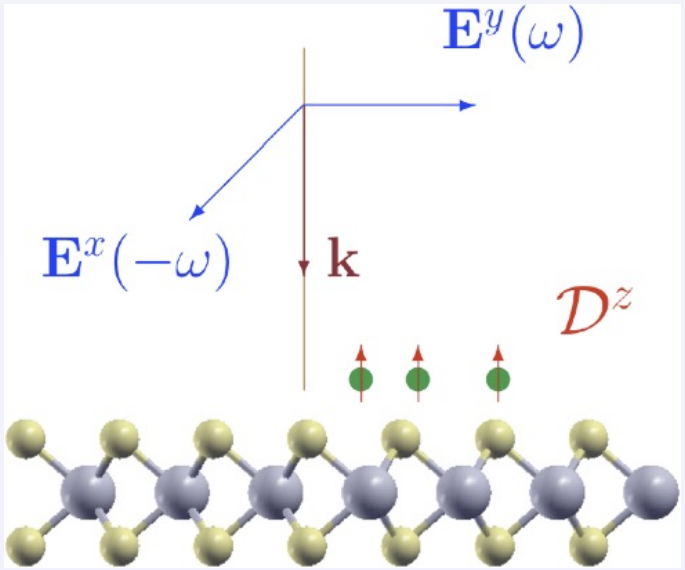
# *Theory*

The DSP in the direction $a$ is given by

$$\mathcal{D}^a(\ell,\omega) = \frac{\dot{\mathcal{S}}^a(\ell,\omega)}{(\hbar/2)\dot{n}(\ell,\omega)}.$$

The incident optical electric field is circularly polarized

$$\mathbf{E}(\omega) = E_0(\omega)(\hat{x} + i\hat{y})/\sqrt{2}.$$



## Spin generation rate

$$\dot{S}^{a}(\ell;\omega) = \zeta^{abc}(\ell;\omega)E^{b}(-\omega)E^{c}(\omega)$$

## Rate of generation of charge carriers

$$\dot{n}(\ell;\omega) = \xi^{ab}(\ell;\omega)E^{a}(-\omega)E^{b}(\omega)$$

$$\begin{aligned}\zeta^{abc}(\ell,\omega) &= \frac{\pi e^2}{\hbar^2}\int\frac{d\mathbf{k}}{8\pi^3}\sum_{cc'v}\mathcal{S}^{a}_{c'c}(\ell,\mathbf{k})r^{b}_{vc'}(\mathbf{k})r^{c}_{cv}(\mathbf{k}) \\ &\times \left[\delta(\omega-\omega_{cv}(\mathbf{k}))+\delta(\omega-\omega_{c'v}(\mathbf{k}))\right] \qquad (1)\end{aligned}$$

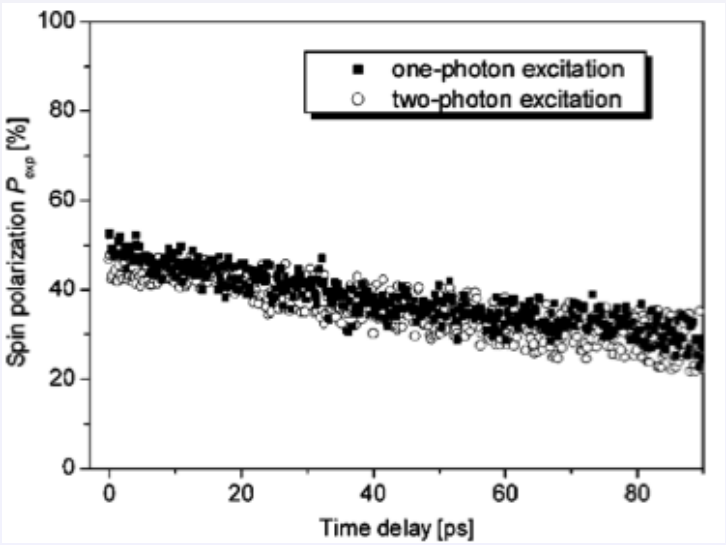
$$\begin{aligned}\xi^{ab}(\ell;\omega) &= \frac{\pi e^2}{\hbar^2}\int\frac{d\mathbf{k}}{8\pi^3}{\sum_{vcc'}}'\mathrm{Re}\left[\varrho_{c'c}(\ell;\mathbf{k})r^{a}_{vc'}(\mathbf{k})r^{b}_{cv}(\mathbf{k})\right. \\ &+ \left.\varrho_{cc'}(\ell;\mathbf{k})r^{a}_{vc}(\mathbf{k})r^{b}_{c'v}(\mathbf{k})\right]\delta(\omega_{cv}(\mathbf{k})-\omega) \qquad (2)\end{aligned}$$

$c$ and $c'$ are cuasidegenerate conduction bands ($\sim$ 30 meV)

# *Results*

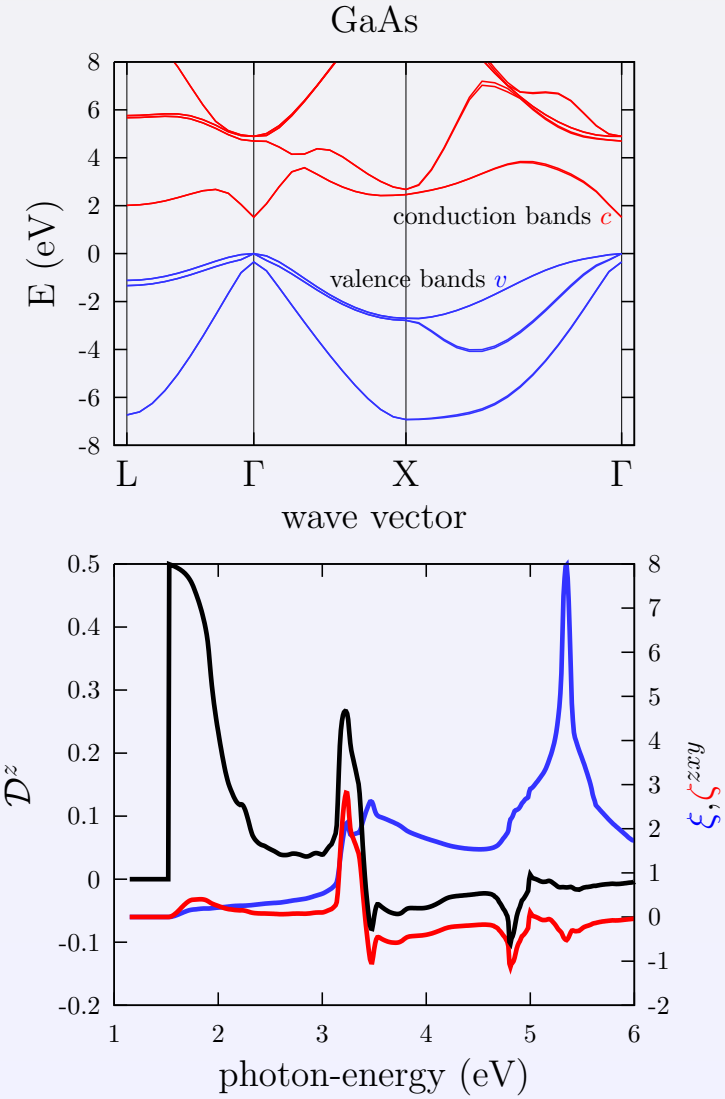
## DSP in bulk GaAs

### Experiment

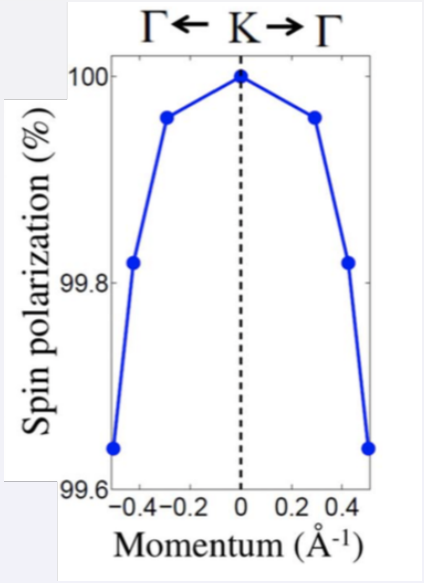


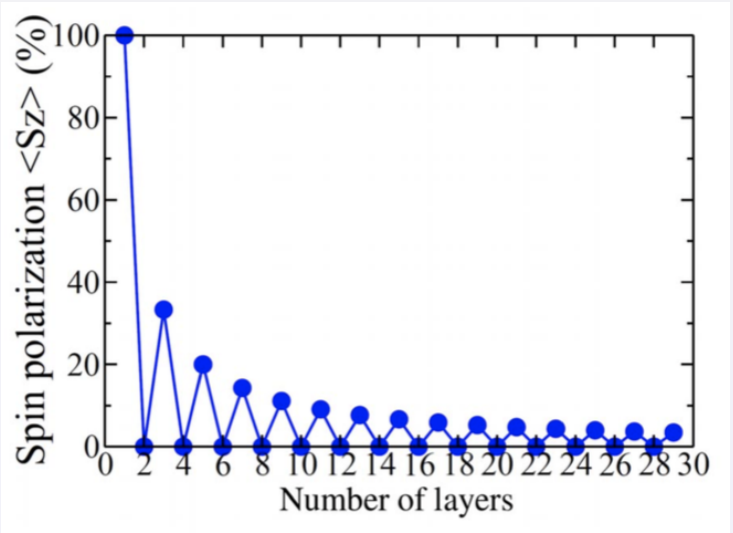

Bhat et al., PRB **71** (2005)

### Theory



# DSP - $MoS_2$-ML




**K** and **K**′ have opposite sign in the DSP, which is ruled by the time reversal symmetry

$$E(\mathbf{k},\uparrow) = E(-\mathbf{k},\downarrow)$$

- Chang et al. considered that DSP is equal to zero in ML structures with an even number of layers since they are CS. Chang et al., Scientific Reports **4**, 6270 (2014).
- For ML structures with an odd number of layers N, they considered that DSP varied as 1/N.

## *Dresselhaus effect*

G. Dresselhaus et al., Phys. Review **100**, 580 (1955).

- Dresselhaus estudied the SO effects in zincblende crystals (GaAs, InSb, CdTe).
- The SOC generates a field $\mathbf{B}_{eff} \sim [\nabla V(\mathbf{r}) \times \mathbf{p})]$, which leads to the spin-splitting of the bands and spin polarization.
- He reported an anisotropic spin splitting of the bands in non CS systems.

## *Rashba effect*

E.I. Rashba and V.I. Sheka, Fiz. Tverd. Tela: Collected papers **2**, 162-76 (1959).
G. Bihlmayer et al., New J. Phys. **17**, 050202 (2015).

- Rashba and Sheka reported that the spin splitting of the bands of wurtzite hexagonal systems corresponding to *s* electrons at around Γ is linear and isotropic in the wave vector **k** perpendicular to the *c* axis.

# *Spin polarization in CS systems*

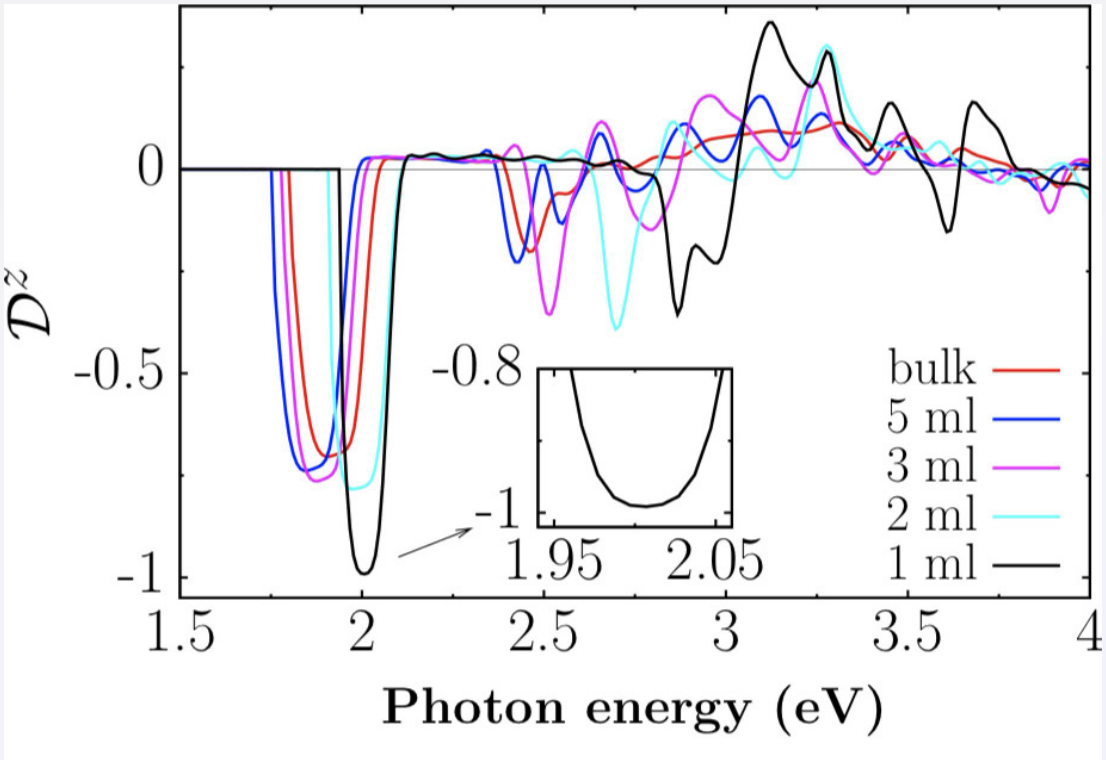
- Considering the Dresselhaus and Rashba effects, it is expected that a 3D material does not have inversion symmetry in order to present spin splitting, and thus spin polarization

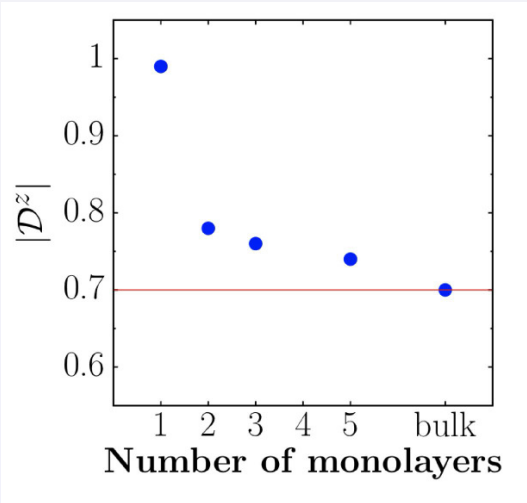
**_Compensated spin polarization_**

X. Zhang. et al. Nature Physics, **10**, 387 (2014).

- Zhang et al. showed that the local symmetry of the system determine the SO interaction
- They reported that, in CS media, though all bands are degenerated, there are two components of the degenerated bands that can have opposite spin polarization corresponding to sectors of the system that mutually present inversion.
- Compensated spin polarization can occur in CS systems with spatial groups $P6_3/mmc$ (e.g. $MoS_2$), $R\bar{3}m$ y $P4/nmm$.

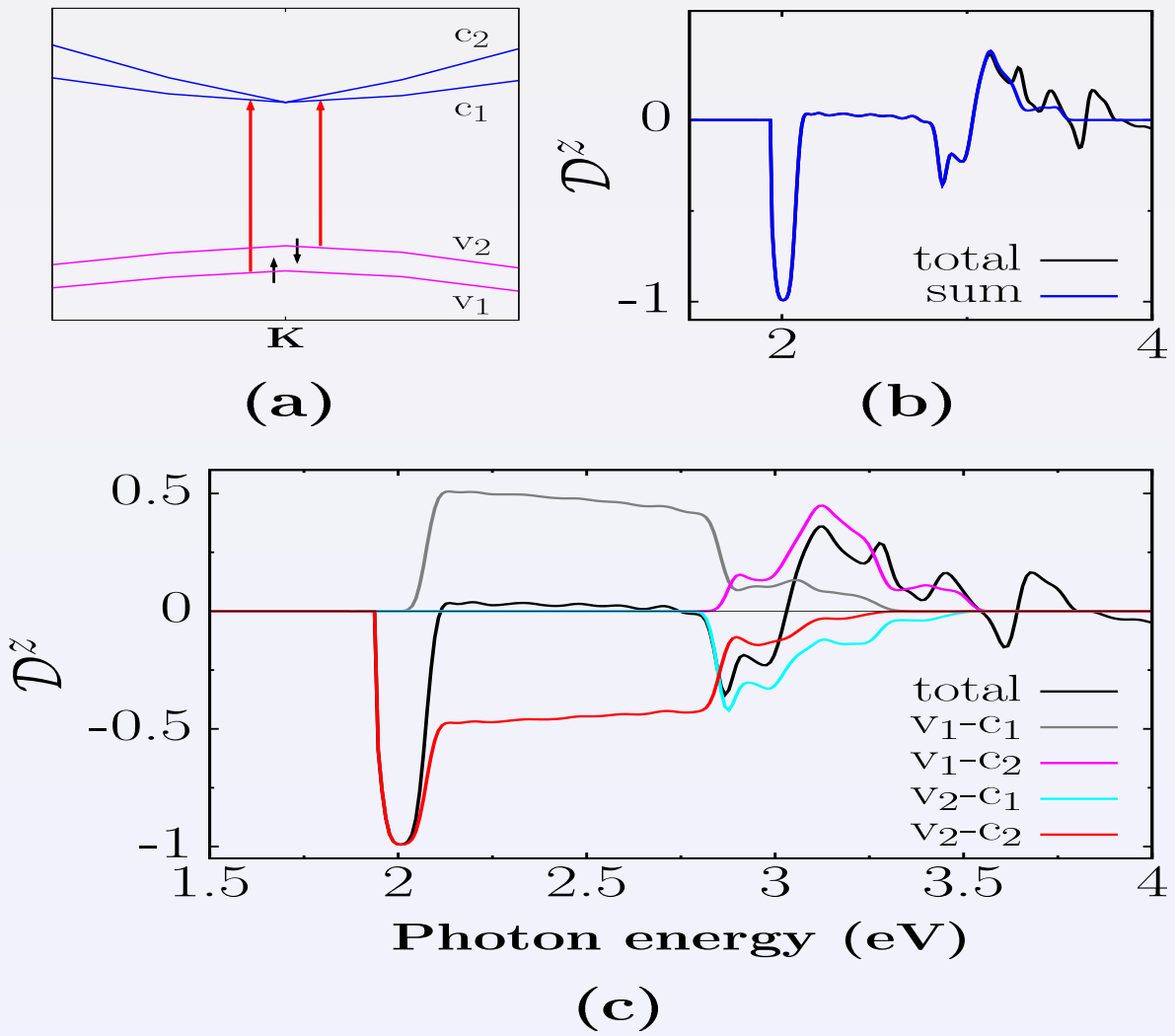
# DSP - $MoS_2$-ML *Arzate et al., PRB* **93**, *115433 (2016).*



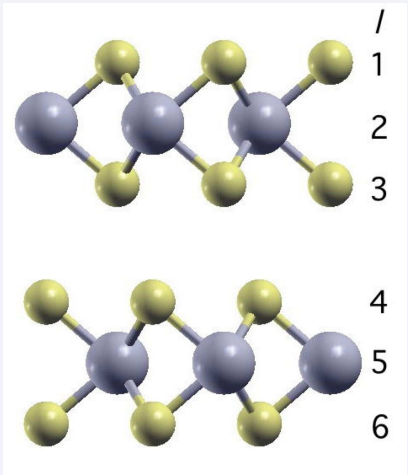

- Calculus of DSP in the whole BZ.
- Convergence with 2912 (392) **k** points in the IBZ in $MoS_2$ ML (bulk) structures.
- Cut off energy of 40 Ha.

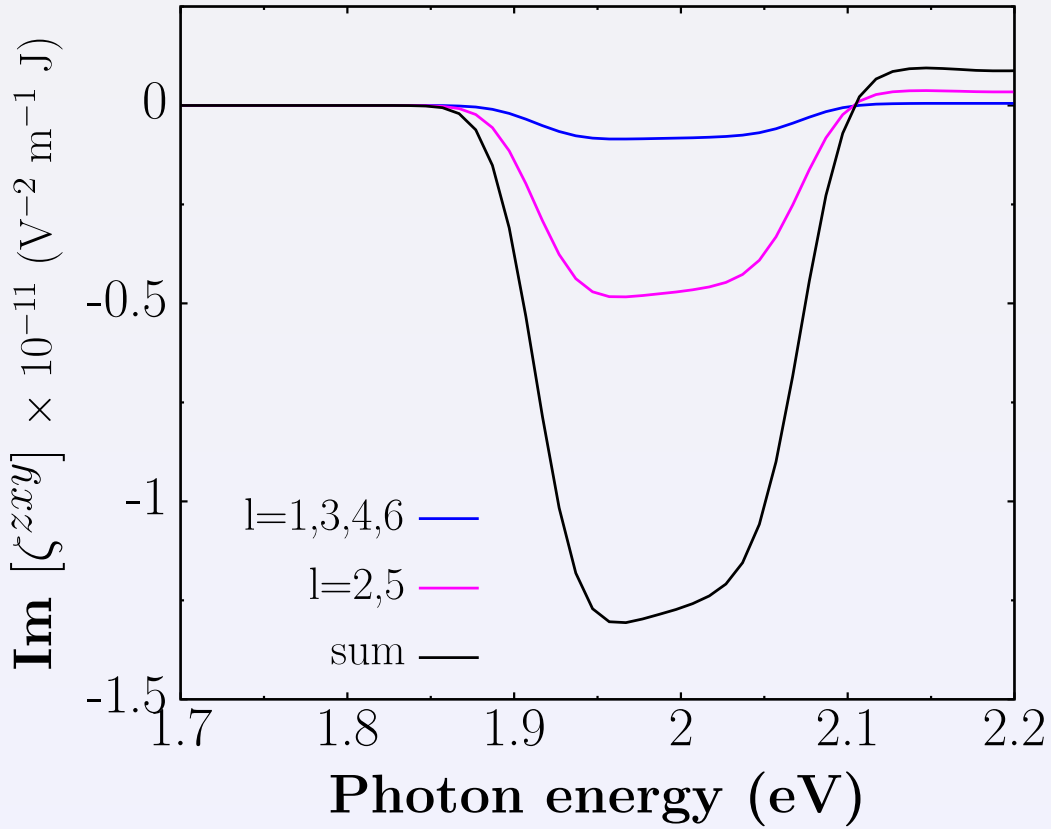
# DSP - $MoS_2$-ML




Arzate et al., PRB **93**, 115433 (2016).

# *Spin generation - $MoS_2$-ML*




Arzate et al., PRB **93**, 115433 (2016).

# DSP - *Comparison*

| System | Energy (eV) | $\lvert\mathcal{D}_z\rvert$ (%) | Reference |
|---|---|---|---|
| 1-ml $MoS_2$ | 2.01 | 100 | Arzate 2016 |
| Bulk $MoS_2$ | 1.91 | 70 | Arzate 2016 |
| $C_{16}H_8$-alt | 0.72 | 22 | Zapata-Peña 2016 |
| Si(111)-In 8×2 | 0.74 | 32 | Arzate 2014 |
| Si(111)-In 4×2 | 0.64 | 30 | Arzate 2014 |
| Si(111)-In $\sqrt{3} \times \sqrt{3}$ R30$^o$ | 2.00 | 44 | Mendoza 2012 |
| Si(111)-As 1×1 | 2.20 | 100 | Mendoza 2012 |
| GaAs(110)-clean 1×1 | 1.64 | 90 | Mendoza 2012 |
| GaAs(110)-Sb 1×1 | 0.84 | 52 | Mendoza 2012 |
| Bulk Si | 3.44 | 30 | Nastos 2007 |
| Bulk Ge | 0.90 | 50 | Rioux 2010 |
| Bulk GaAs | 1.50 | 50 | Nastos 2007, Bhat 2005 (exp) |
| Bulk CdSe | 1.80 | 100 | Nastos 2007 |

## *Summary*

- We have teoretically studied the optical response and spin injection of atomic monolayer of $MoS_2$ structures

## *Conclusions*

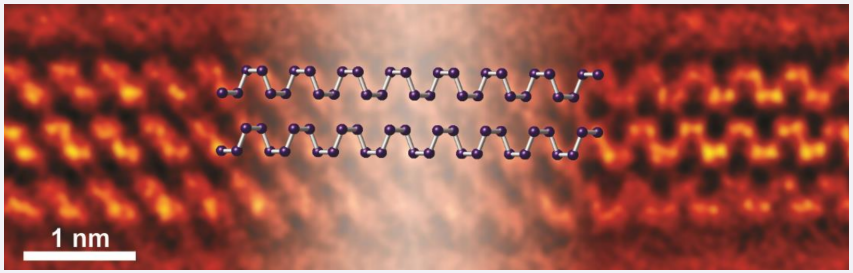
- It is possible to inject spin-polarized electrons into the conduction bands of molybdenum disulfide monolayer structures with circularly polarized light.
- The DSP of the $MoS_2$ ML is of 100% at the photon energy of 2.01 eV corresponding to the transition energy at the **K** point.
- As the number of monolayers increases, the maximum value of DSP decreases to the bulk value of 70 % a 1.91 eV.
- The $MoS_2$ monolayer structures are potential materials to be used for spintronics applications.

# *Phosphorous and Phosphorene*

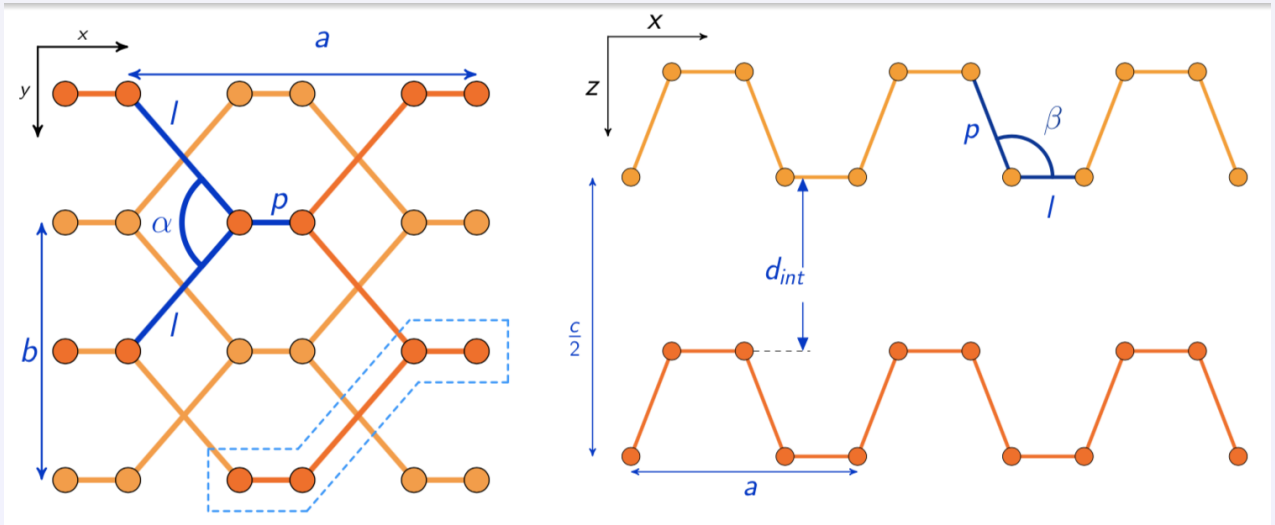
## *Black Phosphorous (BP)*

- Allotropic forms of phosphorous: black, violet, red, and white, in different cristalline structures. [Karttunen et al. Chem. Phys. **9** 2550, (2008), Brown et al. Acta Cristal. **19**, 684 (1965)].
- Most stable phases of BP: orthorrombic (semiconductor), rombhoedric (semimetal) and cubic (metal) [Liu et al. Chem. Soc. Reviews, **44** 2732 (2015)].
- The semiconductor BP belongs to the spatial group Cmca (# 64) and arrange in atomic monolayers.

# *Phosphorene*



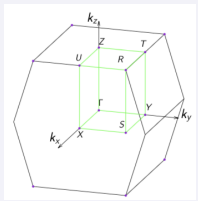

a) STEM image of bulk BP. Space group #64 mmm. [R. J. Wu, et al., Microscopy and Microanalysis **21**, 109 (2015)].

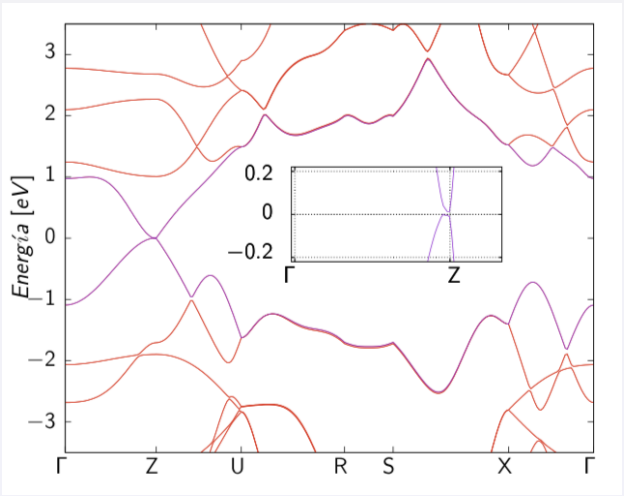


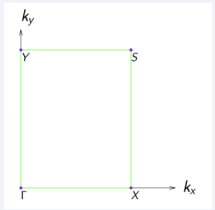

Schematic of top and side views of 2 ML phosphorene. Space group #53 mmm

# *Band structure of BP and phosphorene*

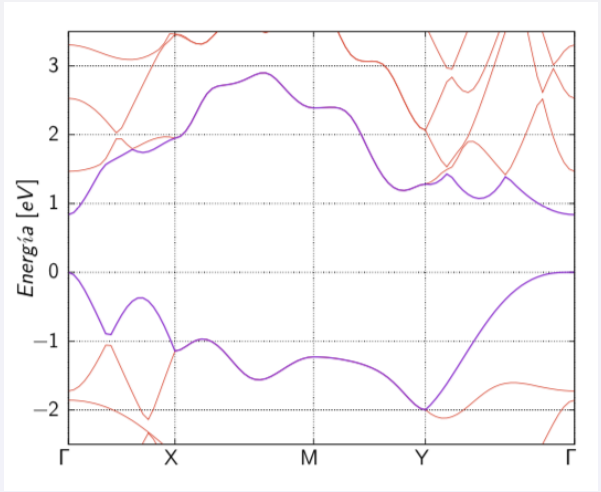
(a) BP





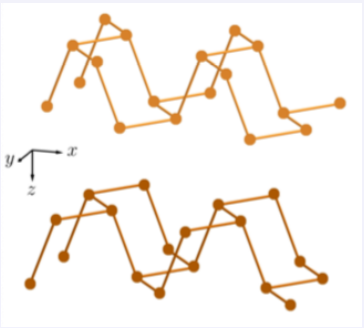

(b) Phosphorene

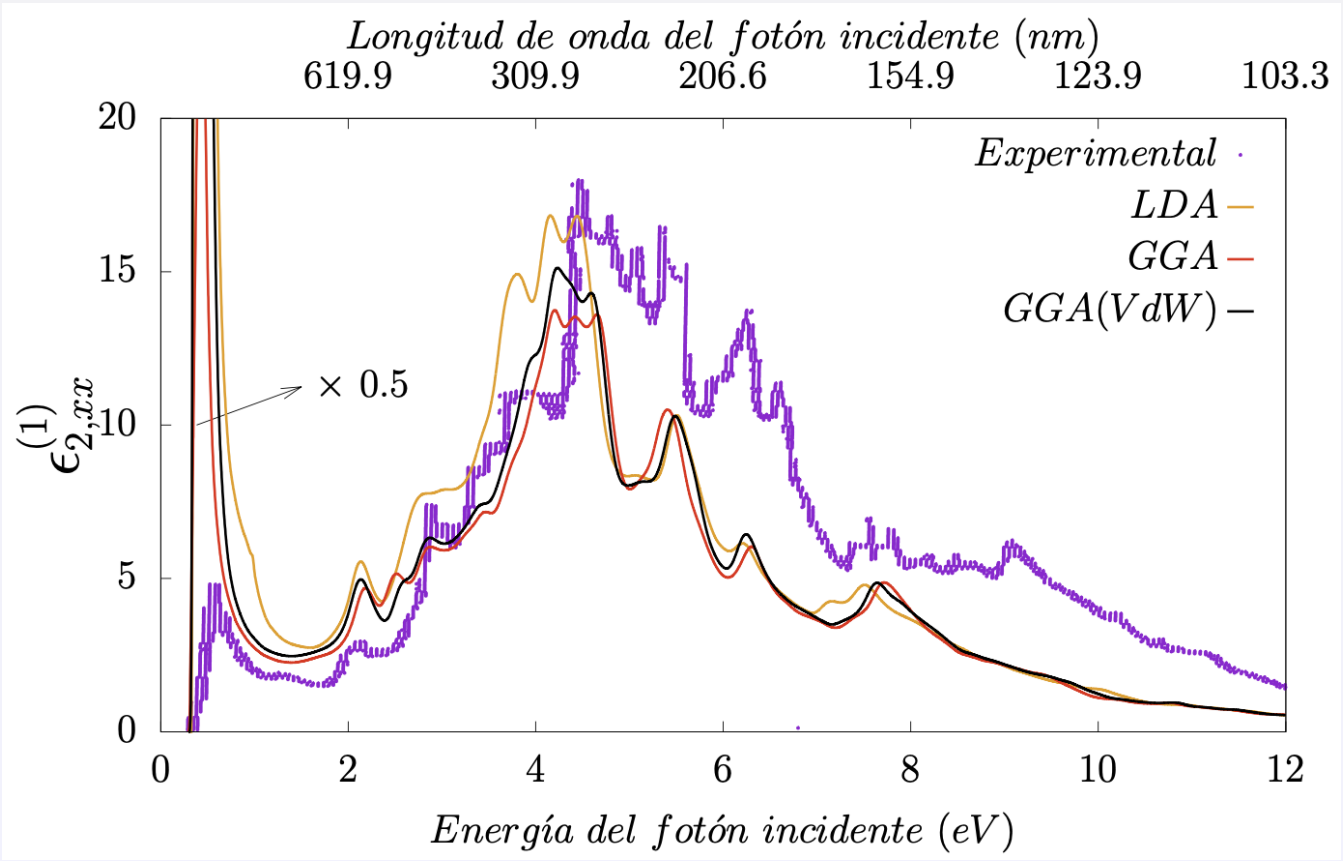



Structural parameters

| | a (Å) | b (Å) | c (Å) | Band gap (eV) |
|---|---|---|---|---|
| BP | | | | |
| LDA | 4.34 | 3.21 | 5.35 | 0.10 |
| GGA | 4.49 | 3.31 | 5.53 | 0.02 |
| GGA(VdW) | 4.44 | 3.28 | 5.47 | 0.08 |
| Phosphorene | | | | |
| LDA | 4.34 | 3.20 | | 0.60 |
| GGA | 4.49 | 3.31 | | 0.84 |

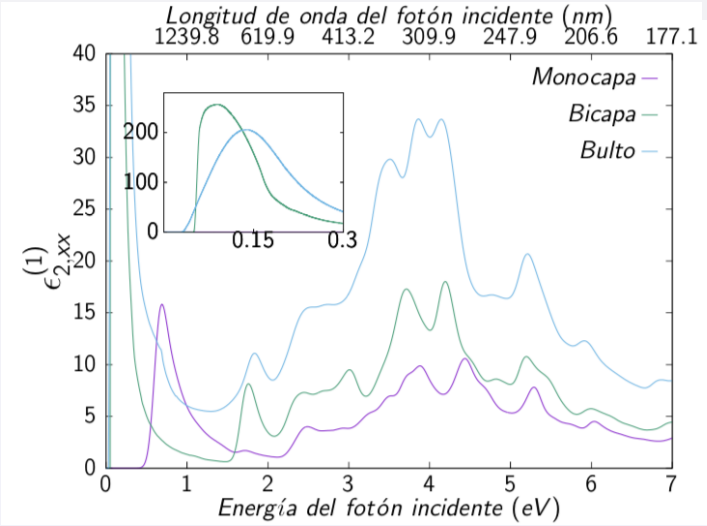
# *Dielectric function of BP - comparison with experiment*

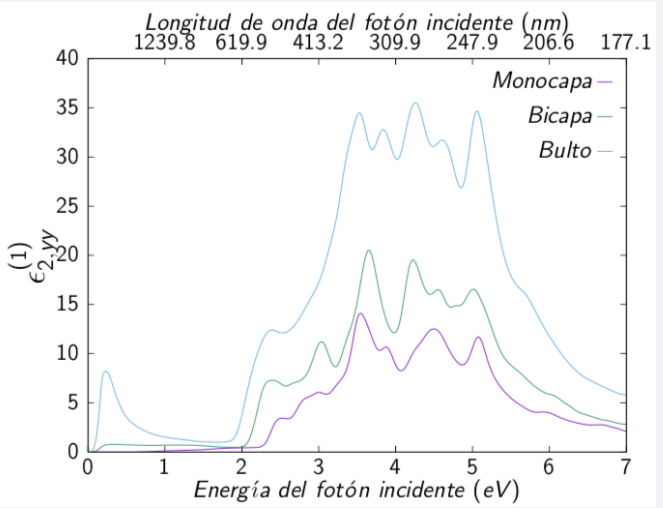


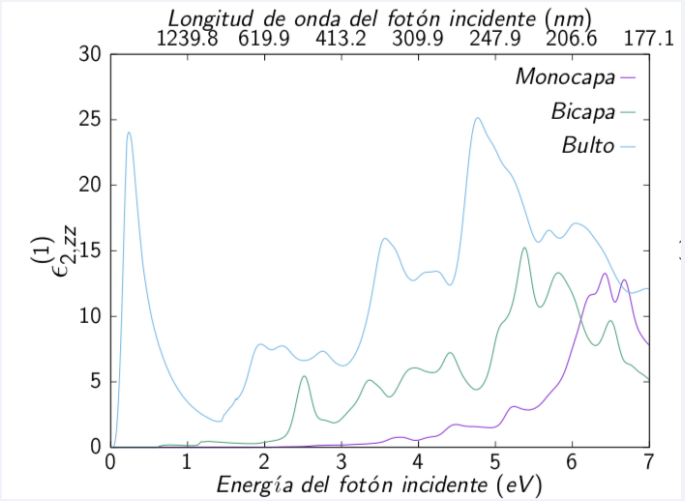



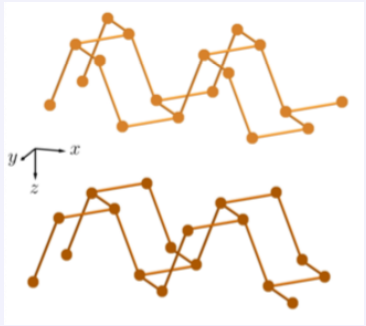

[H. Asahina and A. Morita, J. Phys. C: Solid State Phys. **17**, 1839 (1984)]

# *Dielectric function of BP and phosphorene*




- Phosphorous and phosphorene are semiconductors:
  $E^{\mathrm{BP}}_{\mathrm{exp}} = 0.30$ eV;
  $E^{\mathrm{BP}}_{\mathrm{lda-gap}} = 0.10$ eV;
  $E^{\mathrm{bilayer}}_{\mathrm{lda-gap}} = 0.05$ eV;
  $E^{\mathrm{ML}}_{\mathrm{lda-gap}} = 0.60$ eV

- The dielectric function is anisotropic and depends on the kind of structure monolayer, bilayer and bulk BP.

## *Summary*

- We have studied the linear optical response of black Phosphorous and phosphorene.
- We have calculated the electronic band structure and the imaginary part of the dielectric function of black Phosphorous and phosphorene.

## *Conclusion*

- Both the Black Phosphorous and phosphorene present a highly anisotropic optical response.
- Overall, the respective linear optical response spectrum decreases as BP goes from the bulk to the one monolayer structure

# Contents

*Introduction*

*Method*

*Atomic monolayers*
- Ferromagnetic layers of $\alpha$-$In_2Se_3$
- Dichalcogenides - Case of $MoS_2$
  - Optical spin injection
- Phosphorene

***Summary and Conclusions***

*Computing facilities*

## *Summary*

- We have studied the atomic ML structures of $\alpha$-$In_2Se_3$, $MoS_2$, and phosphorene through the calculation of their lineal, non linear or spin injection response.

## *General conclusions*

- In general, the linear and nonlinear optical response is sensitive to changes of atomic structure and thicknesses of atomic MLs.
- Atomic monolayers of $MoS_2$ can be used for spintronics applications. In particular, it is possible to tailor the degree of spin polarization as a function of ML thickness by incidence of circularly polarized light.

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*Summary and Conclusions*

***Computing facilities***

# Computing facilities

Acknowledgements: CONACyT - Mexico.

**Cluster**

- 3 Intel Xeon *sixteen-core* nodes of 4U (192 cores) of 64 bits and 3 Tb of RAM p/node.
- 36 Intel Xeon dual *six-core* nodes (432 cores) of 64 bits and 48 Gb of RAM p/node.

Gracias por su atención