Universiteit Antwerpen

Yunnan University

The optoelectronic properties of monolayer MoS_2 in the presence of Rashba spin-orbit coupling

Yiming Xiao[1,2]

1. CMT Group, University of Antwerp
2. Yunnan University, Kunming, China

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Outline

- Low energy band structure of monolayer MoS_2
- The role of Rashba effect
- Optical conductivity of ML-MoS_2 in the presence of Rashba spin-orbit coupling
- The infrared to terahertz optical absorption
- Conclusion

Band structure of monolayer MoS_2

Experimentally fabricated in 2010:

Phys. Rev. Lett. 105, 136805 (2010)
ACS Nano 4, 2695 (2010).

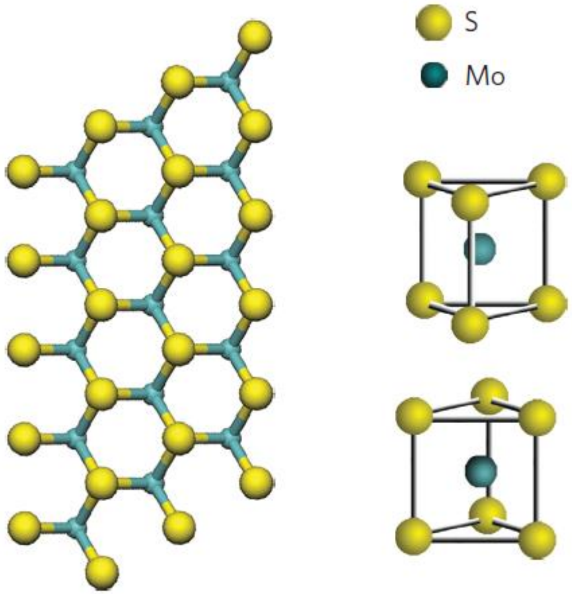


Fig. 1 Schematic of MoS_2 monolayer structure

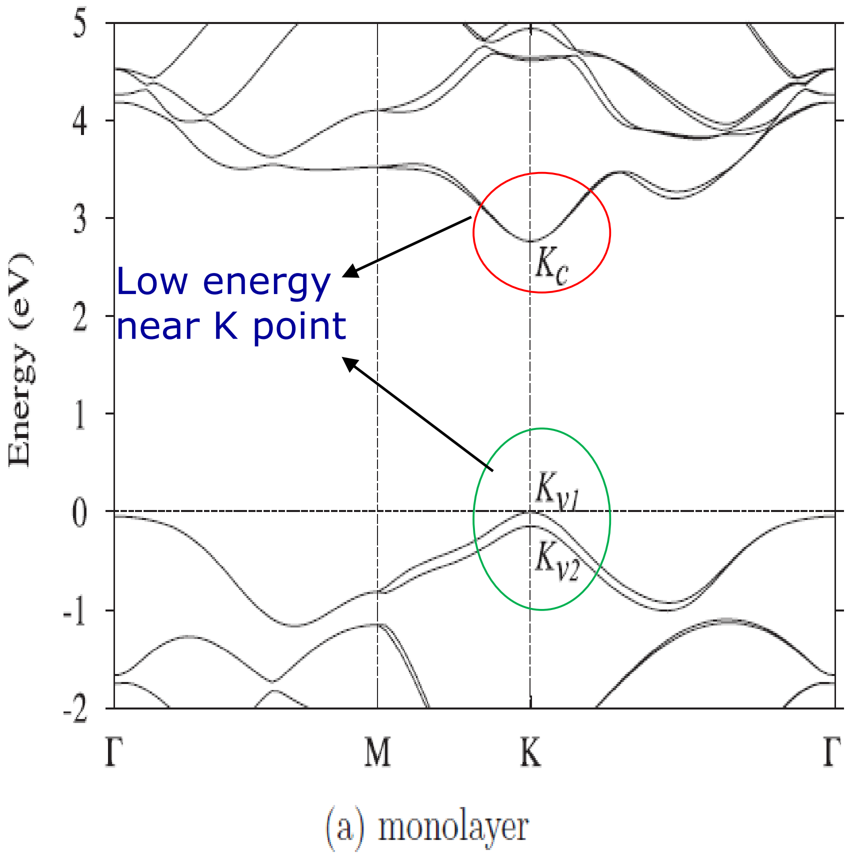


Fig. 2 Band structures of monolayer MoS_2

Phys. Rev. B 85, 205302 (2012)

Low energy bandstructure

Effective low energy k · p hamiltonian

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

Massive Dirac fermions

$$\hat{H}^{\varsigma} = [at(\varsigma k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) + \frac{\Delta}{2}\hat{\sigma}_z]$$

$$+ \varsigma \gamma_v \frac{\hat{I} - \hat{\sigma}_z}{2} \hat{s}_z$$

Valley

Intrinsic SOC

$$\hat{H}_0^{\varsigma} = \begin{pmatrix} \Delta/2 & \varsigma a t k_{-\varsigma} \\ \varsigma a t k_{\varsigma} & -\Delta/2 + \varsigma s \gamma_v \end{pmatrix}$$

$$E_{\lambda \mathbf{k}}^{\varsigma s} = \varsigma s \gamma/2 + \lambda [a^2 t^2 k^2 + \Delta_{\varsigma s}^2]^{1/2}$$

Parabolic band behavior:

Taylor expansion around k=0

$$\tilde{E}_{\lambda \mathbf{k}}^{\varsigma s} = \lambda \frac{a^2 t^2 \mathbf{k}^2}{2\Delta_{\varsigma s}} + \lambda \Delta_{\varsigma s} + \frac{\varsigma s \gamma}{2}$$

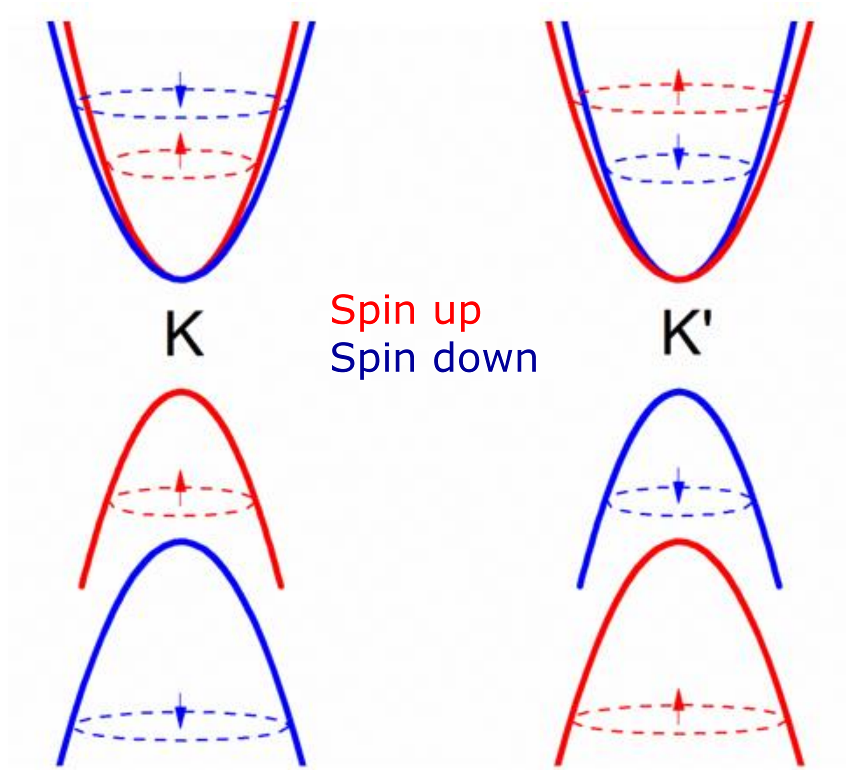


Fig. 3 Low energy band structures of monolayer MoS_2

Spin is decoupled $\hat{s}_z$ *is good quantum number*

Transition between blue and red band: forbidden

How to make the optical response in this regime?

The Rashba effect

A electrical field E_z create it
By gate voltage or substrate

$$\hat{H}^{\varsigma} = [at(\varsigma k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) + \frac{\Delta}{2}\hat{\sigma}_z] \otimes \hat{I} + \varsigma\gamma_v \frac{\hat{I} - \hat{\sigma}_z}{2} \otimes \hat{s}_z + \boxed{\gamma_R(\varsigma\hat{\sigma}_x \otimes \hat{s}_y - \hat{\sigma}_y \otimes \hat{s}_x),}$$

Rashba SOC

$$\hat{H}^{\varsigma} = \begin{pmatrix} \Delta/2 & 0 & \varsigma atk_{-\varsigma} & 0 \\ 0 & \Delta/2 & 2i\gamma_R & \varsigma atk_{-\varsigma} \\ \varsigma atk_{\varsigma} & -2i\gamma_R & \gamma_v - \Delta/2 & 0 \\ 0 & \varsigma atk_{\varsigma} & 0 & -\gamma_v - \Delta/2 \end{pmatrix}$$

Eigenfunction：4 components vector

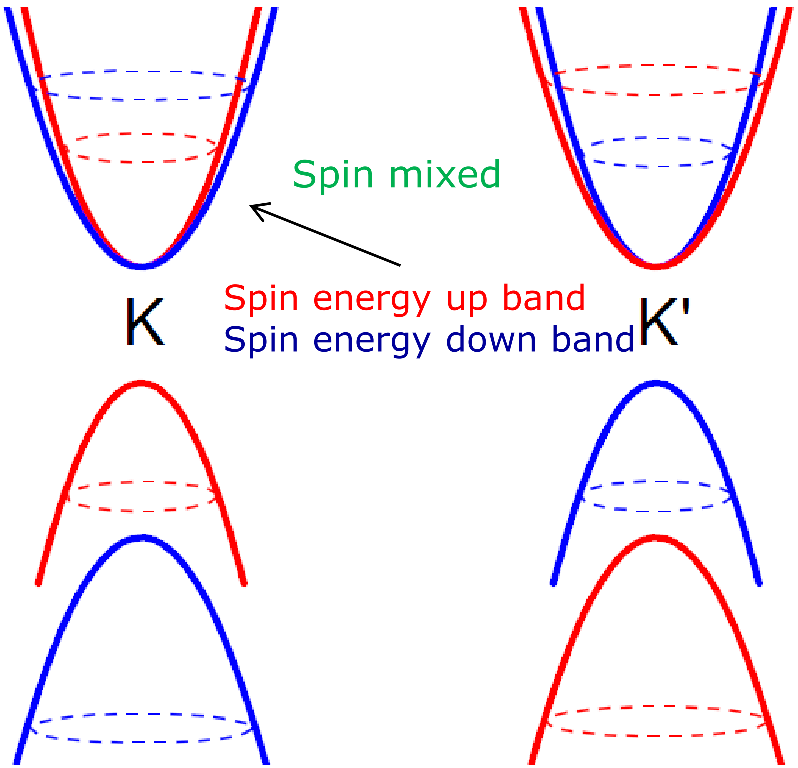


Fig. 3 band structures in the presence of Rashba SOC

Rashba effect mixes the spin states
Spin index is not good a quantum number

Transition between blue and red band: possible
Optical matrix elements

Phys. Rev. Lett. 108, 196802 (2012).
Phys. Rev. B 87, 245421 (2013).

Optical conductivity: theoretical approach

Kubo-Greenwood formula:

$$\sigma^{\varsigma}_{\alpha\beta}(\omega) = \frac{ie^2}{\omega} \sum_{\lambda' s', \lambda s} \sum_{\mathbf{k}', \mathbf{k}} \boxed{\langle \mathbf{k}, \xi | \hat{v}^{\varsigma}_{\alpha} | \mathbf{k}', \xi' \rangle \langle \mathbf{k}', \xi' | \hat{v}^{\varsigma}_{\beta} | \mathbf{k}, \xi \rangle}$$

Optical matrix elements

Large gap ⟶ $\lambda' = \lambda$

$$\times \frac{f(\varepsilon_{\mathbf{k},\xi}) - f(\varepsilon_{\mathbf{k}',\xi'})}{\varepsilon_{\mathbf{k},\xi} - \varepsilon_{\mathbf{k}',\xi'} + \hbar(\omega + i\eta)},$$

the velocity operator $\hat{v}^{\varsigma}_{\alpha} = \hbar^{-1} \partial \hat{H}^{\varsigma} / \partial k_{\alpha}$.

Total optical conductivity: $\sigma_{\alpha\beta}(\omega) = \sum_{\varsigma = \pm} \sigma^{\varsigma}_{\alpha\beta}(\omega)$

Real part of longitudinal conductivity:

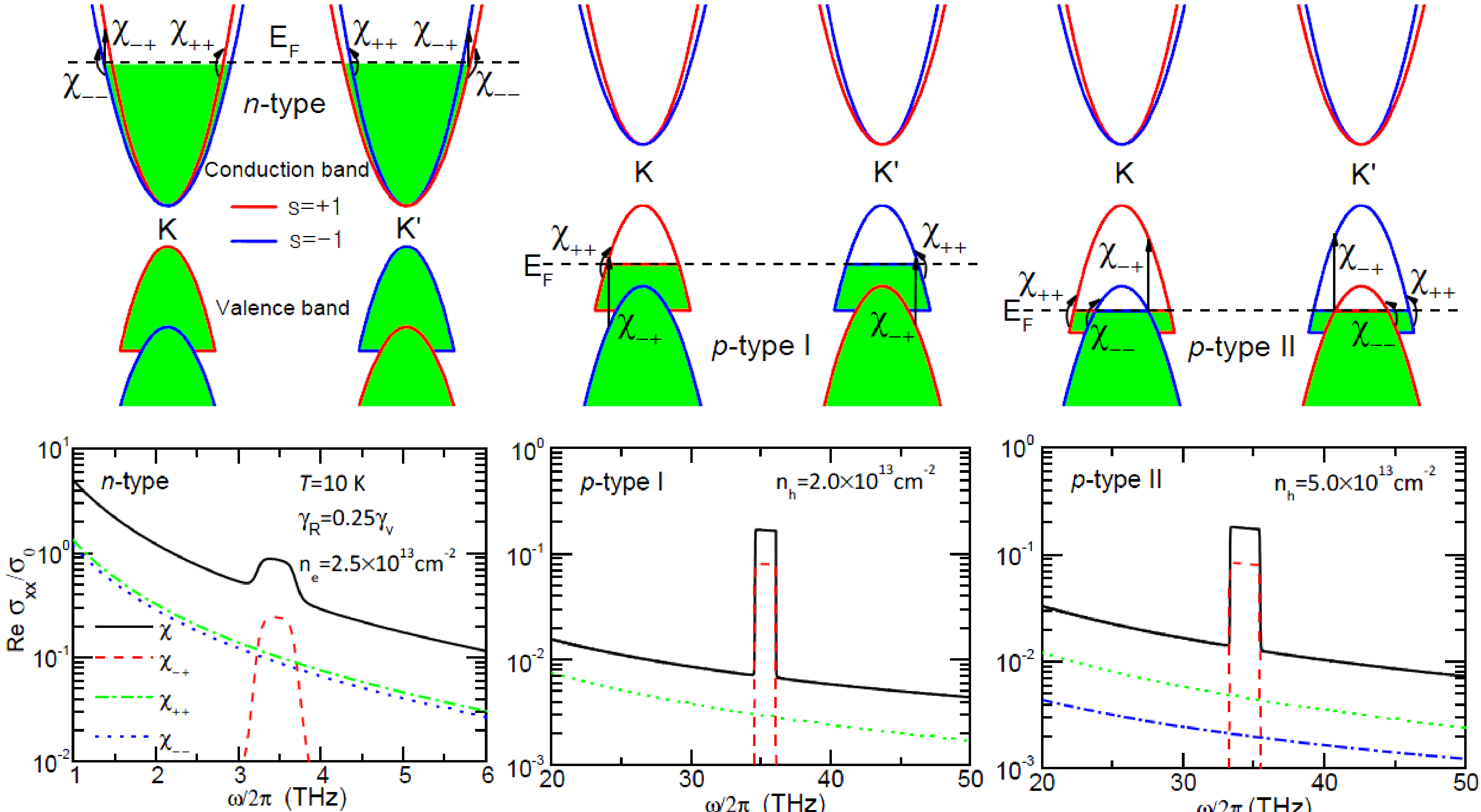
1. Intra-band and inter-band transitions
2. Independent on valley index ⟶ Valley degenerate

Imaginary of transverse conductivity

1. Intra-band transitions: is zero
2. Inter-band transitions: none zero valley index dependent

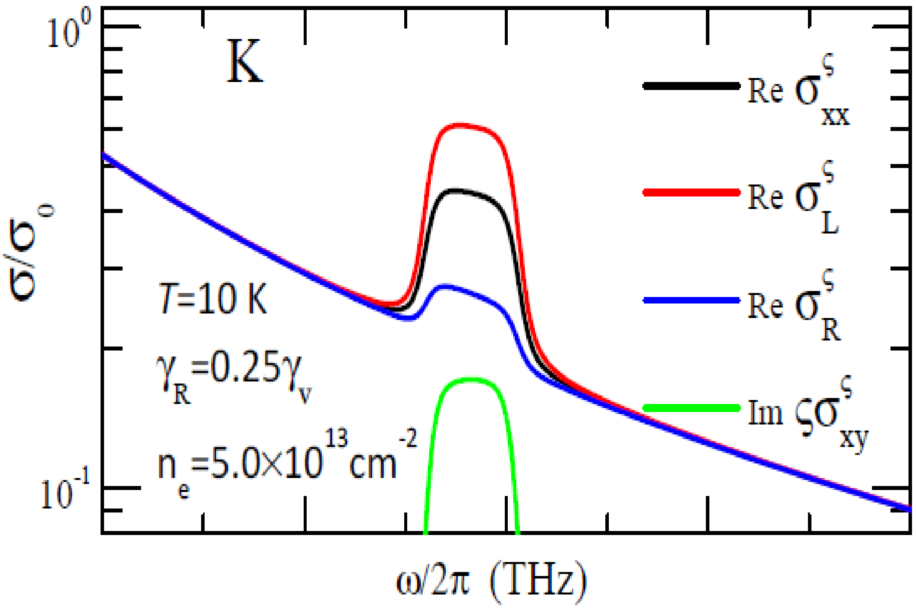
Condensed Matter Physics (Wiley, New York, 2000)
Phys. Rev. B 87, 125425 (2013).

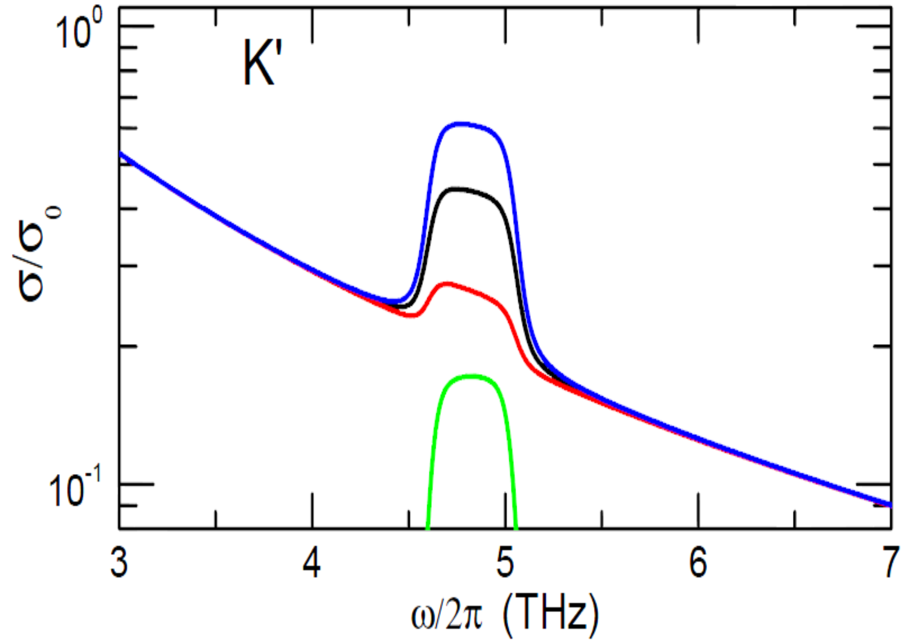
Optical absorption channels



The optical conductivity as a function of frequency

Valley selective circular light absorption





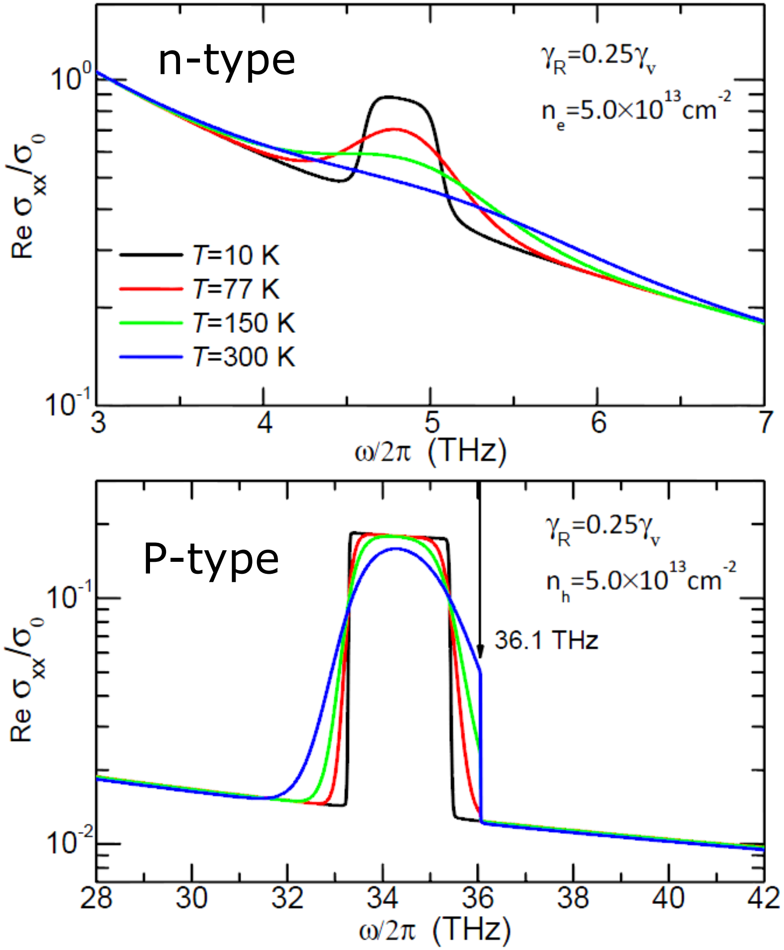
Valley dependent Hall conductivity: $\mathrm{Im}\ \sigma_{xy}^{+}(\omega) = -\mathrm{Im}\ \sigma_{xy}^{-}(\omega)$

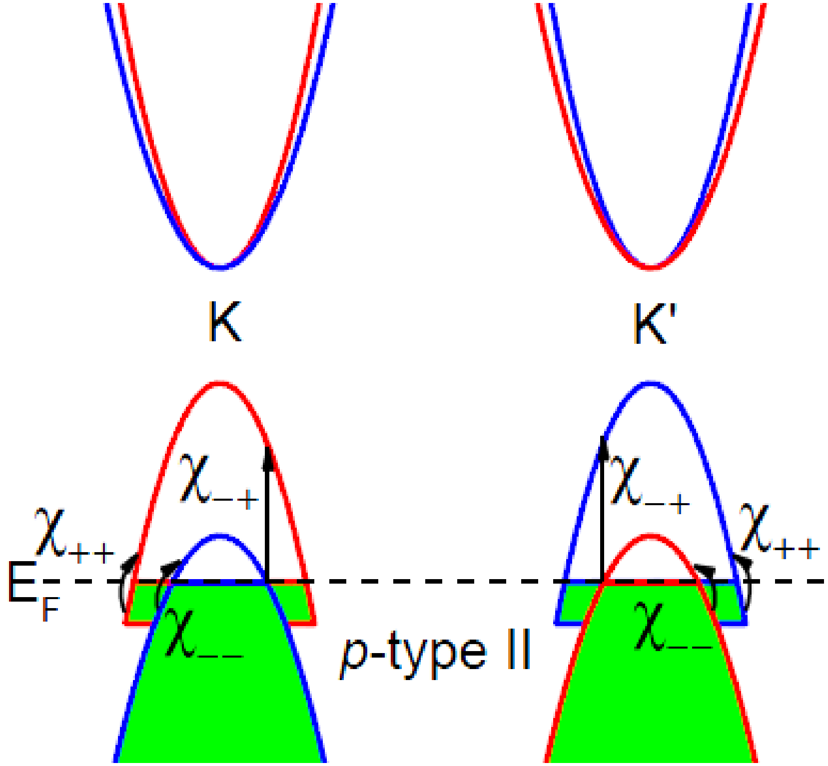
Absorption under circular polarized light:

$$\mathrm{Re}\ \sigma_{\mathrm{L}}^{\varsigma}(\omega) = \mathrm{Re}\ \sigma_{xx}^{\varsigma}(\omega) + \mathrm{Im}\ \sigma_{xy}^{\varsigma}(\omega)$$

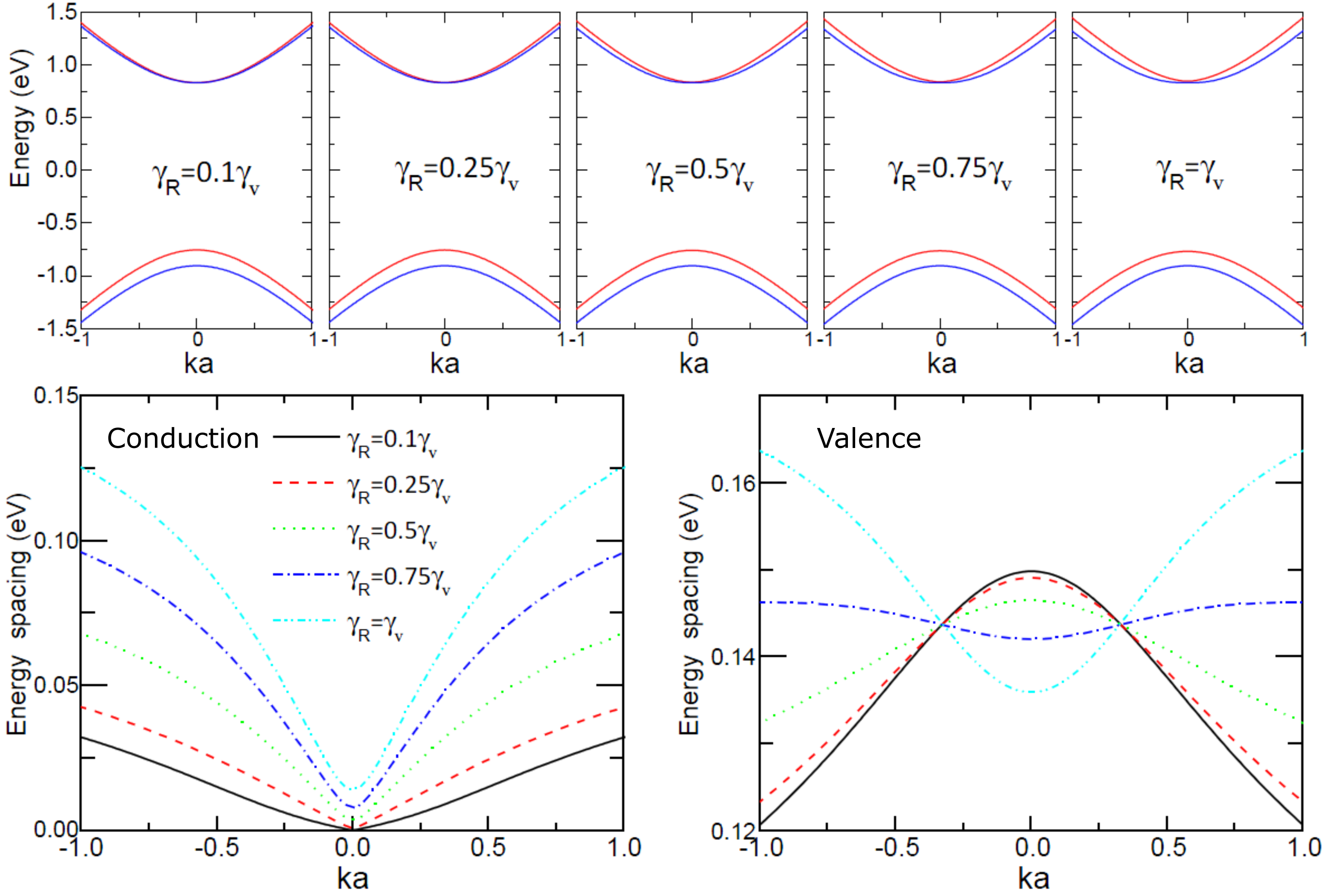
$$\mathrm{Re}\ \sigma_{\mathrm{R}}^{\varsigma}(\omega) = \mathrm{Re}\ \sigma_{xx}^{\varsigma}(\omega) - \mathrm{Im}\ \sigma_{xy}^{\varsigma}(\omega)$$

The effect of temperature on absorption

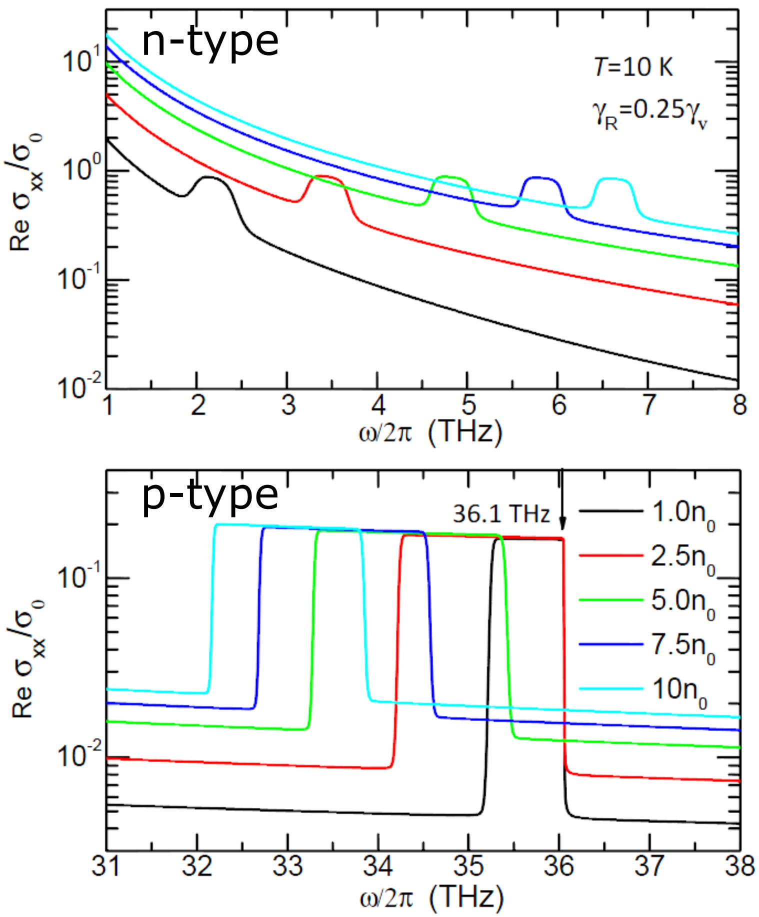




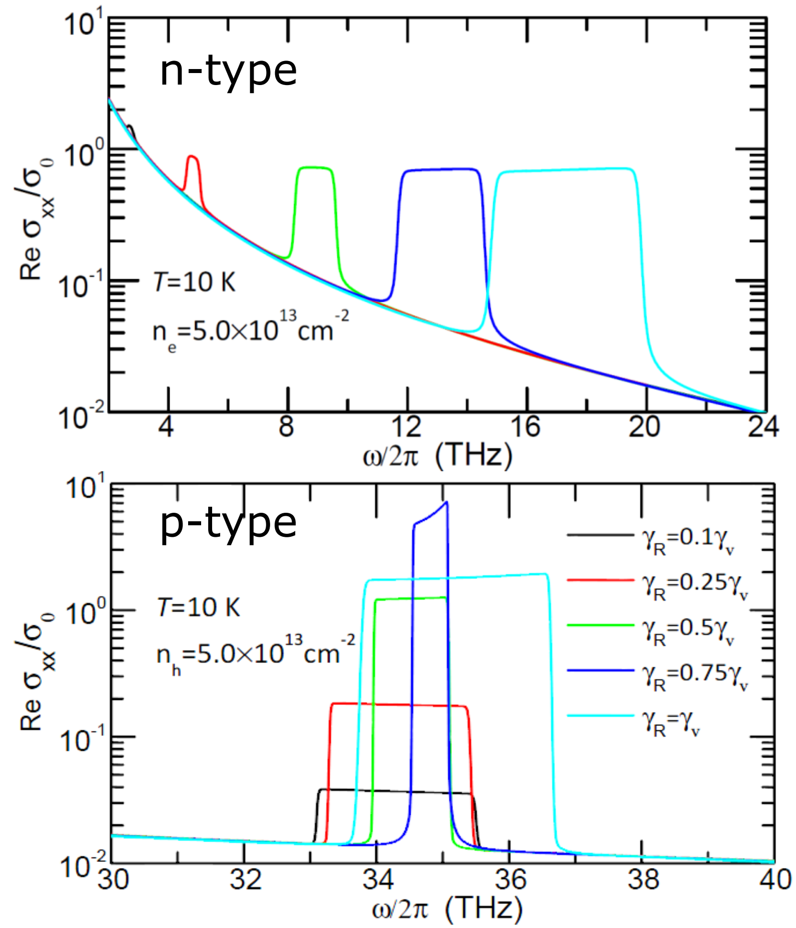
The Rashba effect tuned band structure



Optical absorption's tunability



Carrier density's tunability



Rashba strength's tunability via electrical field

The absorption window can be tuned by carrier density and Rashba parameter

Conclusions

- Rashba effect induced spin-flip transitions have wide absorption peaks or absorption windows which range from infrared to THz.
- Under circularly polarized radiation, the spin-flip transitions have a valley selective absorption.
- The position and width of the absorption peak and absorption window can be effectively tuned by carrier density and Rashba strength.
- Monolayer MoS_2 can be a promising tunable optical and optoelectronic material that is active in the infrared to terahertz spectral range.

Thanks for your attention!