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The Valley Hall Effect in MoS_2 Transistors

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arXiv:1403.5039 [cond-mat.mes-hall]

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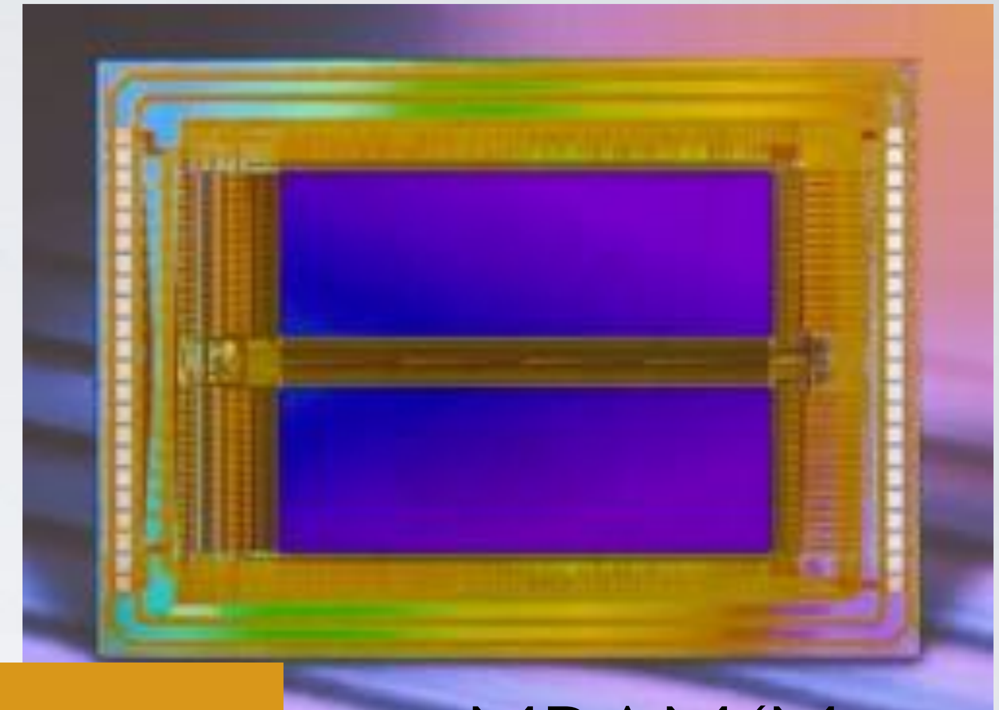
Electronics

Spintronics



MRAM(Motorola)

Valleytronics

?

Prospective

Outline

1. Anomalous velocity
2. The valley Hall effect
3. Valley-selective circular dichroism of monolayer MoS_2
4. The valley Hall effect in MoS_2 transistors

1. Anomalous velocity

Berry curvature

parameter set

$$\Omega^n_{\mu\nu} = i\left[\left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \middle| \frac{\partial n(\mathbf{R})}{\partial R^\nu} \right\rangle - (\nu \leftrightarrow \mu)\right]$$

$|n(\mathbf{R})\rangle$: instantaneous eigenstates of Hamiltonian at each value of $\mathbf{R}$

i.e.

$$H(\mathbf{R})\,|n(\mathbf{R})\rangle = \varepsilon_n(\mathbf{R})\,|n(\mathbf{R})\rangle$$

Hamiltonian and eigenstates

Independent electron approximation

periodic potential with $\mathbf{a}$

$$H = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r})$$

band index

Bloch's theorem: $\psi_{n,\mathbf{q}}(\mathbf{r}+\mathbf{a}) = e^{i\mathbf{q}\cdot\mathbf{a}}\psi_{n\mathbf{q}}(\mathbf{r})$

crystal momentum

$\mathbf{q}$ -dependent Hamiltonian: $H(\mathbf{q}) = e^{-i\mathbf{q}\cdot\mathbf{r}} H e^{i\mathbf{q}\cdot\mathbf{r}}$

$$= \frac{(\hat{\mathbf{p}}+\mathbf{q})^2}{2m} + V(\mathbf{r})$$

$$u_{n,\mathbf{q}}(\mathbf{r}) = e^{-i\mathbf{q}\cdot\mathbf{r}}\psi_{n\mathbf{q}}(\mathbf{r})$$

parameter space: Brillouin zone, $|u_n(\mathbf{q})\rangle$: basis function

Wave function

$\mathbf{q}(t)$: changes slowly in time

time-dependent Scrhodinger equation: $i \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle$

instantaneous eigenstates

$$|\psi(t)\rangle = \sum_n \exp\left(-i \int_{t_0}^{t} dt' E_n(t') \right) a_n(t) |n(t)\rangle$$

$$\dot{a}_n(r) = -\sum_l a_l(t) \langle n(t)| \frac{\partial}{\partial t} |l(t)\rangle \exp\left(-i \int_{t_0}^{t} dt' [E_l(t') - E_n(t')] \right)$$

First-order wave function

We have an initial condition: $a_n(0) = 1,\ a_{n'} = 0$

For $n' \neq n$

$$\frac{\partial}{\partial t} a_{n'} = -\langle n'| \frac{\partial}{\partial t} |n\rangle \exp\left(-i \int_{t_0}^{t} dt' [E_n(t') - E_{n'}(t')]\right)$$

Integrate by parts

$$a_{n'} = -\frac{\langle n'| \partial/\partial t |n\rangle}{E_n - E_{n'}} i \exp\left(-i \int_{t_0}^{t} dt' [E_n(t') - E_{n'}(t')]\right)$$

$$|\psi(t)\rangle = \exp\left(-i \int_{t_0}^{t} dt' E_n(t')\right) \left\{ |n(t)\rangle - i \sum_{n \neq n'} |n(t)\rangle \frac{\langle n| \partial/\partial t |n\rangle}{E_n - E_{n'}} \right\}$$

The average velocity

Apart from the overall phase factor,

$$|u_n\rangle - i \sum_{n' \neq n} \frac{|n_{n'}\rangle \langle u_{n'}|\, \partial u_n/\partial t\rangle}{\varepsilon_n - \varepsilon_{n'}}$$

velocity operator in the q representation : $v(q,t) = \partial H(q,t)/\partial q$

$$v_n(q) = \frac{\partial \epsilon_n(q)}{\partial q} - i \sum_{n' \neq n} \left\{ \frac{\langle n_n|\, \partial H/\partial q\, |u_{n'}\rangle \langle u_{n'} \partial u_n/\partial t\rangle}{\varepsilon_n - \varepsilon_{n'}} - \text{c.c.} \right\}$$

$$v_n(q) = \frac{\partial \varepsilon_n(q)}{\partial q} - i \underbrace{\left[\left\langle \frac{\partial u_n}{\partial q} \middle| \frac{\partial u_n}{\partial t} \right\rangle - \left\langle \frac{\partial u_n}{\partial t} \middle| \frac{\partial u_n}{\partial q} \right\rangle \right]}_{\textbf{Berry curvature } \Omega^n_{qt}}$$

With electric field

uniform vector potential $A(t)$

$$H(t) = \frac{[\hat{\mathbf{p}} + e\mathbf{A}(t)]^2}{2m} + V(\mathbf{r})$$

q-space $H(\mathbf{q}, t) = H\left(\mathbf{q} + e\mathbf{A}(t)\right)$

gauge invariant crystal momentum: $\mathbf{k} = \mathbf{q} + e\mathbf{A}(t)$

eigenstates: $u_n(\mathbf{k})$

$\mathbf{A}(t)$ preserve the translational symmetry, $\dot{\mathrm{q}} = 0$

$$\dot{\mathbf{k}} = -e\mathbf{E}$$

Anomalous velocity

$$\partial/\partial q_\alpha = \partial/\partial k_\alpha, \ \partial/\partial t = -eE_\alpha \partial/\partial k_\alpha$$

$$v_n(q) = \frac{\partial \varepsilon_n(q)}{\partial q} - \Omega^n_{qt} \quad \Rightarrow \quad \mathbf{v}_n(\mathbf{k}) = \frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}} - \underline{e\mathbf{E} \times \boldsymbol{\Omega}_n(\mathbf{k})}$$

Berry curvature: $\boldsymbol{\Omega}_n(\mathbf{k}) = i \langle \nabla_{\mathbf{k}} u_n(\mathbf{k}) | \times | \nabla_{\mathbf{k}} u_n(\mathbf{k}) \rangle$

anomalous velocity: $-e\mathbf{E} \times \boldsymbol{\Omega}_n(\mathbf{k})$

transverse to the electric field give rise a Hall current

2. The valley Hall effect

Symmetry consideration

$$\mathbf{v}_n(\mathbf{k}) = \frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}} - e\mathbf{E} \times \mathbf{\Omega}_n(\mathbf{k})$$

$$\mathbf{v} \to -\mathbf{v},\ \ \mathbf{k} \to -\mathbf{k},\ \ \mathbf{E} \to \mathbf{E}$$

$$\xrightarrow{\text{time-reversal sym.}} \mathbf{\Omega}_n(-\mathbf{k}) = -\mathbf{\Omega}_n(\mathbf{k})$$

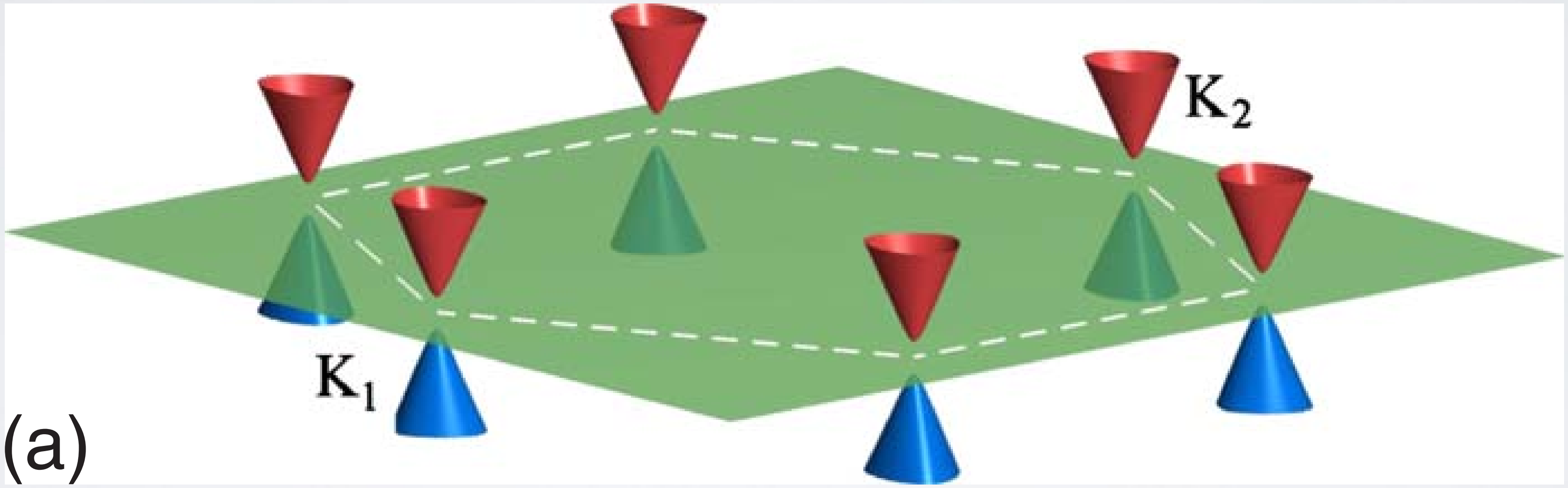
$$\cancel{\mathbf{v} \to -\mathbf{v},\ \ \mathbf{k} \to -\mathbf{k},\ \ \mathbf{E} \to -\mathbf{E}}$$

$$\xrightarrow{\text{spatial inversion sym.}} \cancel{\mathbf{\Omega}_n(-\mathbf{k}) = \mathbf{\Omega}_n(\mathbf{k})}$$

time-reversal and spatial inversion symmetry

$$\Longrightarrow \mathbf{\Omega}_n(\mathbf{k}) = 0$$

2-valley structure



Valley Hall effect

valley index: $\tau_z = \pm 1$

Valley Hall Effect: $\mathbf{j}^v = \sigma_H^v \hat{z} \times \mathbf{E}$

valley Hall conductivity

valley current: $\mathbf{j}^v = \langle \tau_z \mathbf{v} \rangle$

time reversal

$\mathbf{j}^v \to \mathbf{j}^v, \mathbf{E} \to \mathbf{E}$

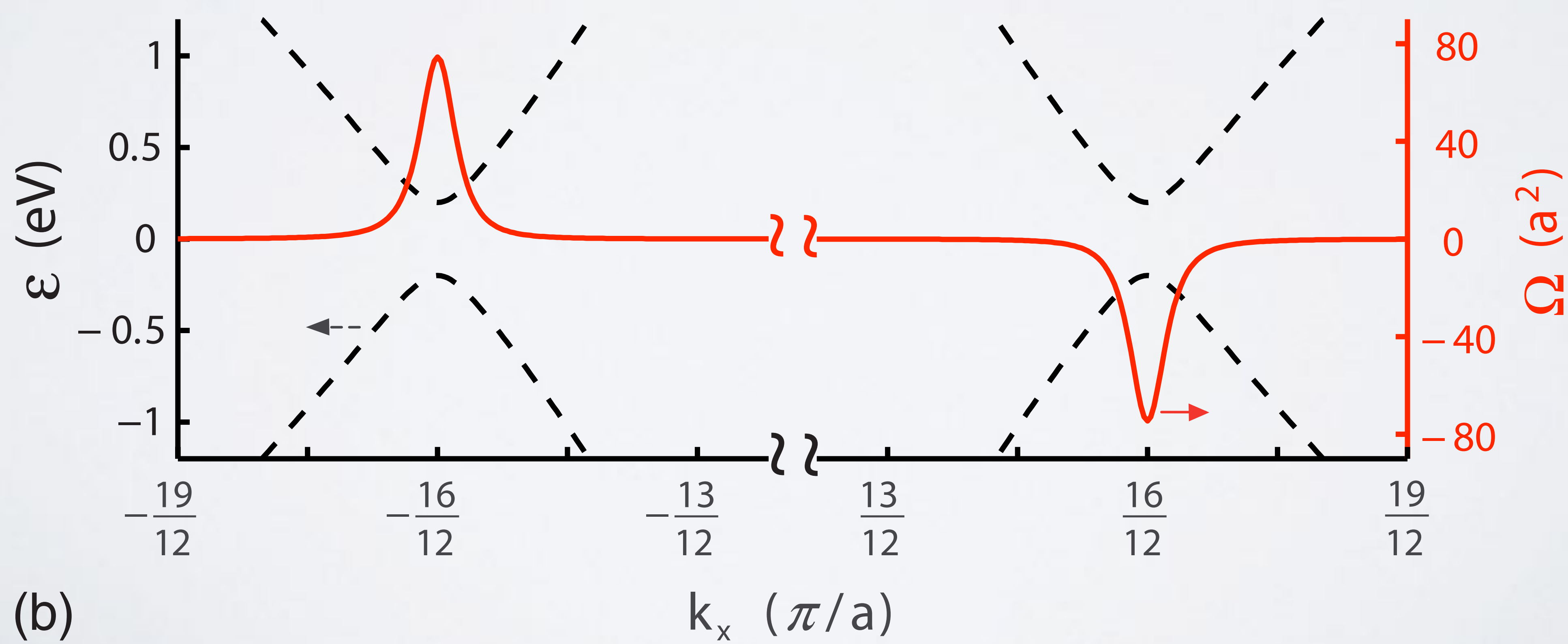
~~inversion symmetry~~

$\mathbf{j}^v \to \mathbf{j}^v, \mathbf{E} \to -\mathbf{E}$

Berry curvature of graphene

In low energy, $H = \frac{\sqrt{3}}{2}at(q_x\tau_z\sigma_x + q_y\sigma_y) + \frac{\Delta}{2}\sigma_z$

$$\Omega(\mathbf{q}) = \tau_z \frac{3a^2t^2\Delta}{2(\Delta^2 + 3q^2a^2t^2)^{3/2}}$$



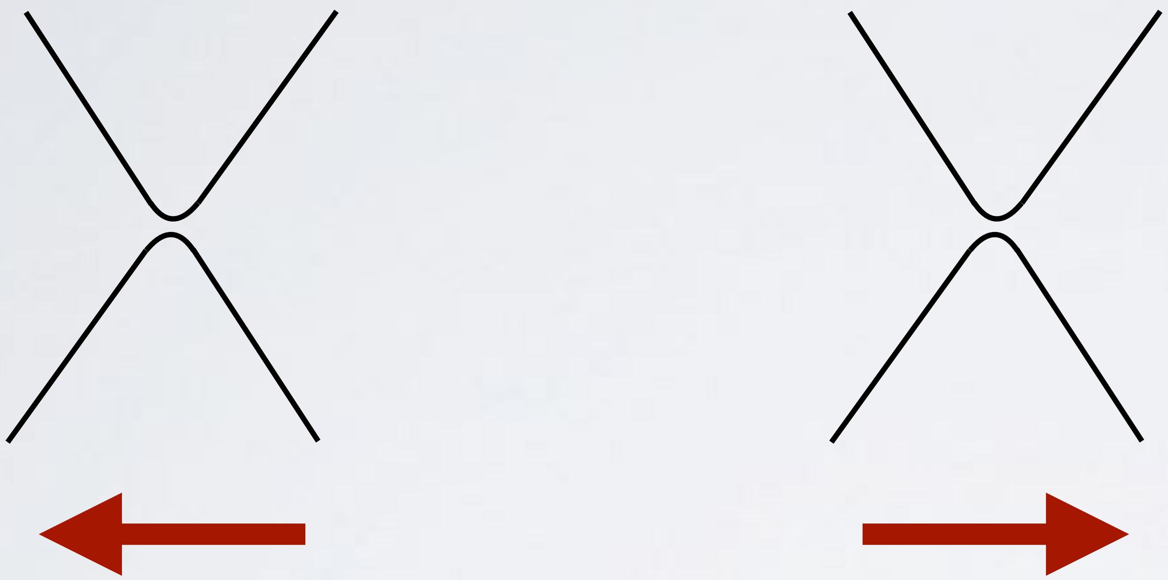
Valley Hall current

Anomalous velocity: $\mathbf{v}_n(\mathbf{k}) = \dfrac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}} - e\mathbf{E} \times \mathbf{\Omega}_n(\mathbf{k})$

$$\begin{aligned} \mathbf{j}^v &= \langle \tau_z \mathbf{v} \rangle \\ &= -2eE \frac{3a^2t^2\Delta}{2(\Delta^2 + 3q^2a^2t^2)^{3/2}} \end{aligned}$$

Valley Hall current!

Pathway to valleytronics



$$\mathbf{j}^C = 0$$

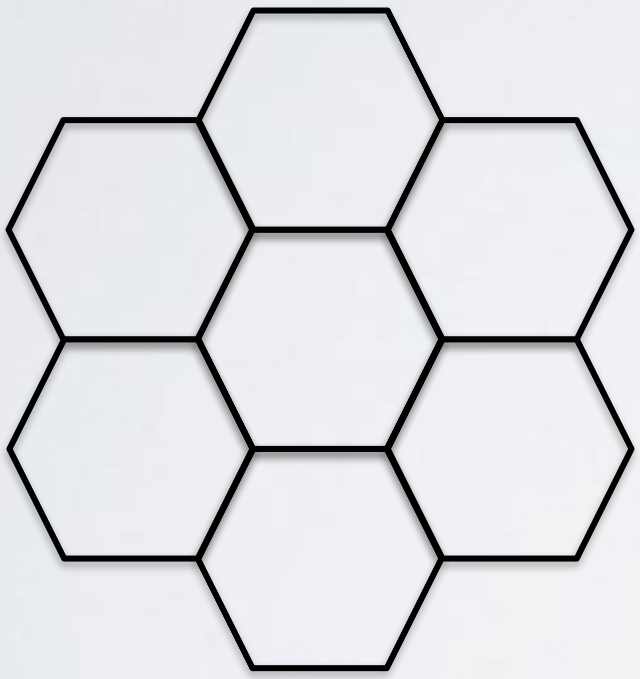
It provides a new and standard pathway to potential applications of valleytronics in a broad class of semiconductors.

3. Valley-selective circular dichroism of monolayer MoS_2

[Ting Cao, Ji Feng, Junren Shi, Qian Niu, Enge Wang,(2012)]

Graphene?

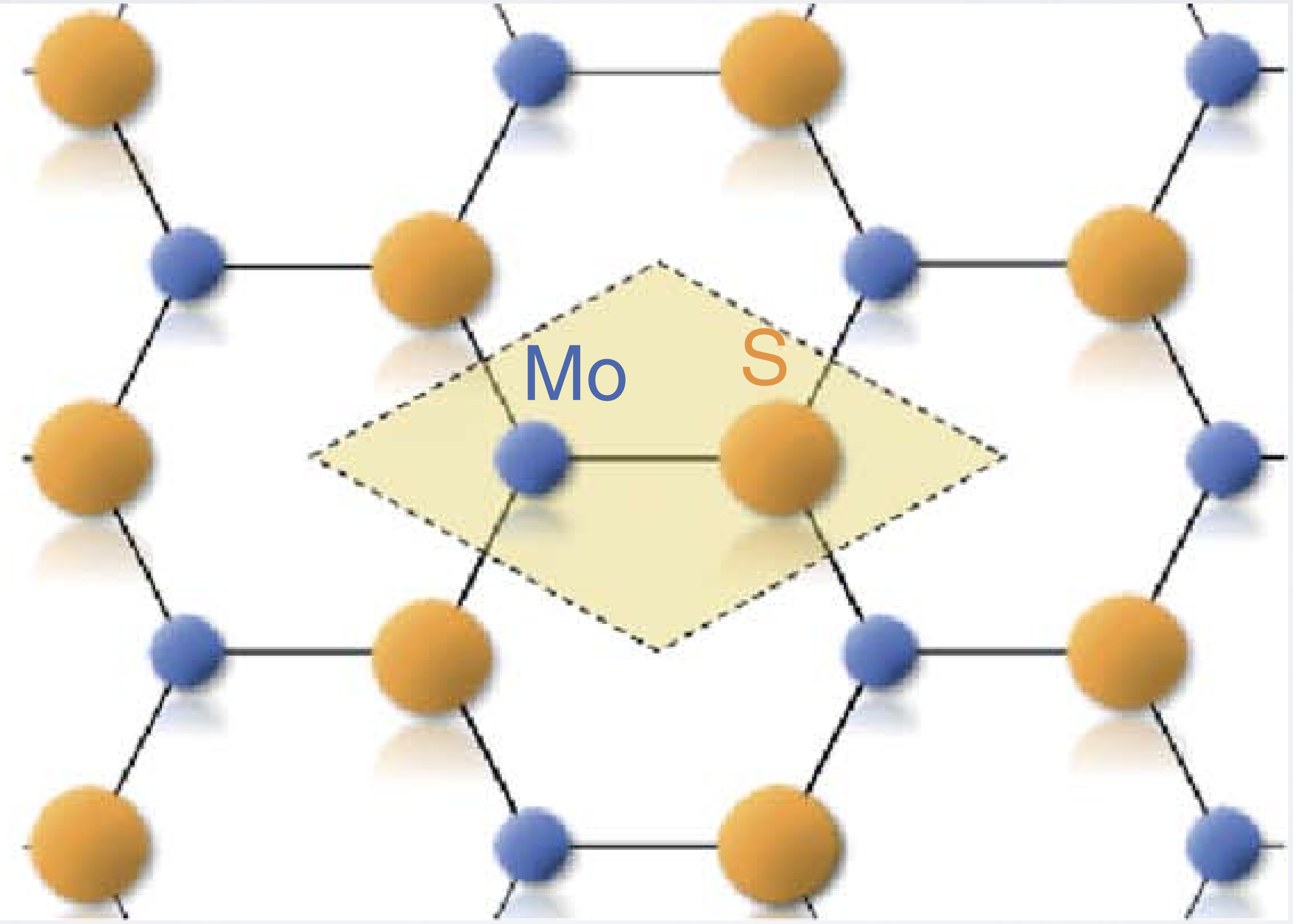
graphene: inversion symmetry



Unprecedented control of the lattice structure on the scale of a single atom is required.

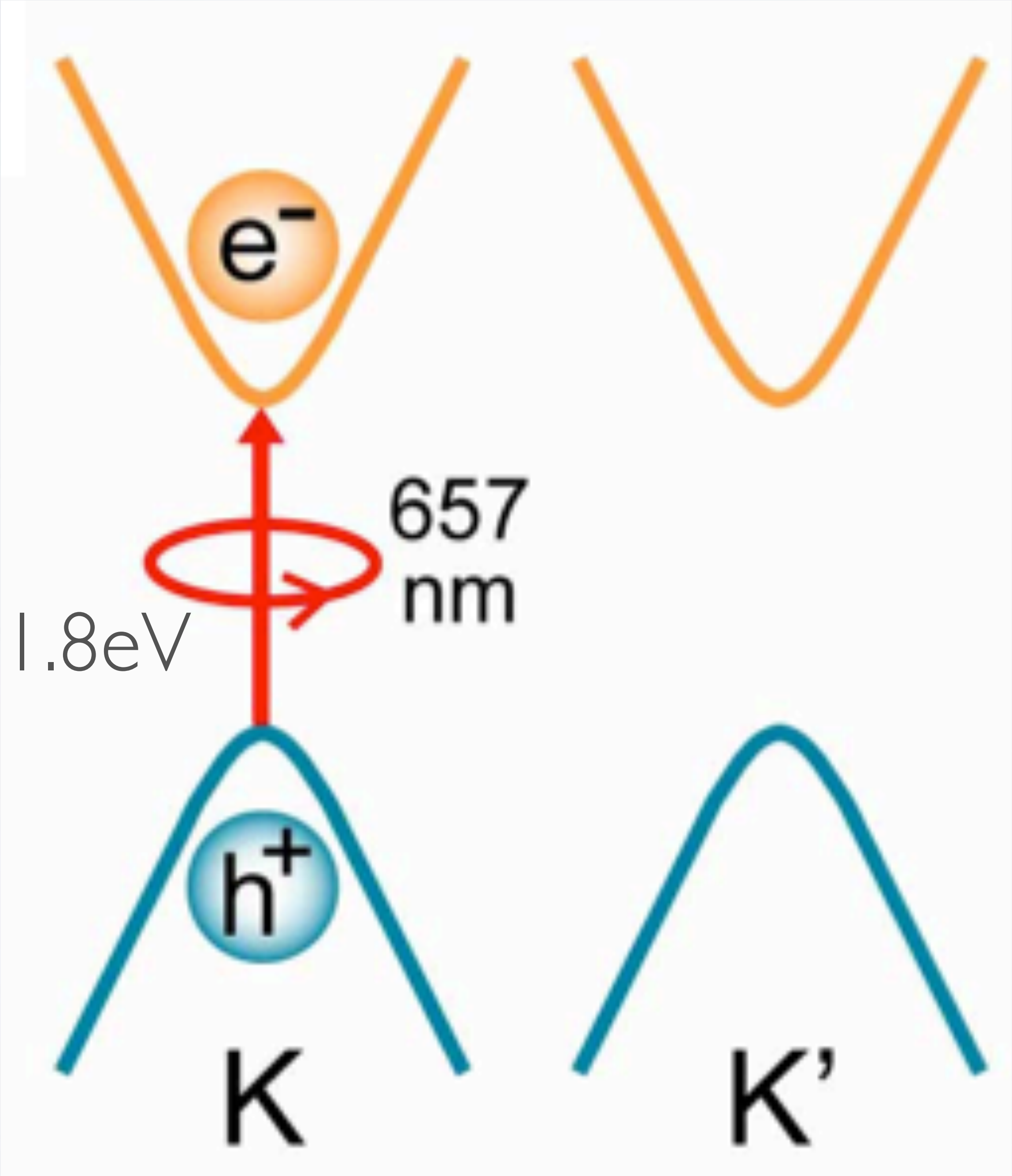
Valleytronics in graphene is very difficult

MoS_2



~~inversion symmetry~~

MoS_2 for valleytronics



Degree of circular polarization

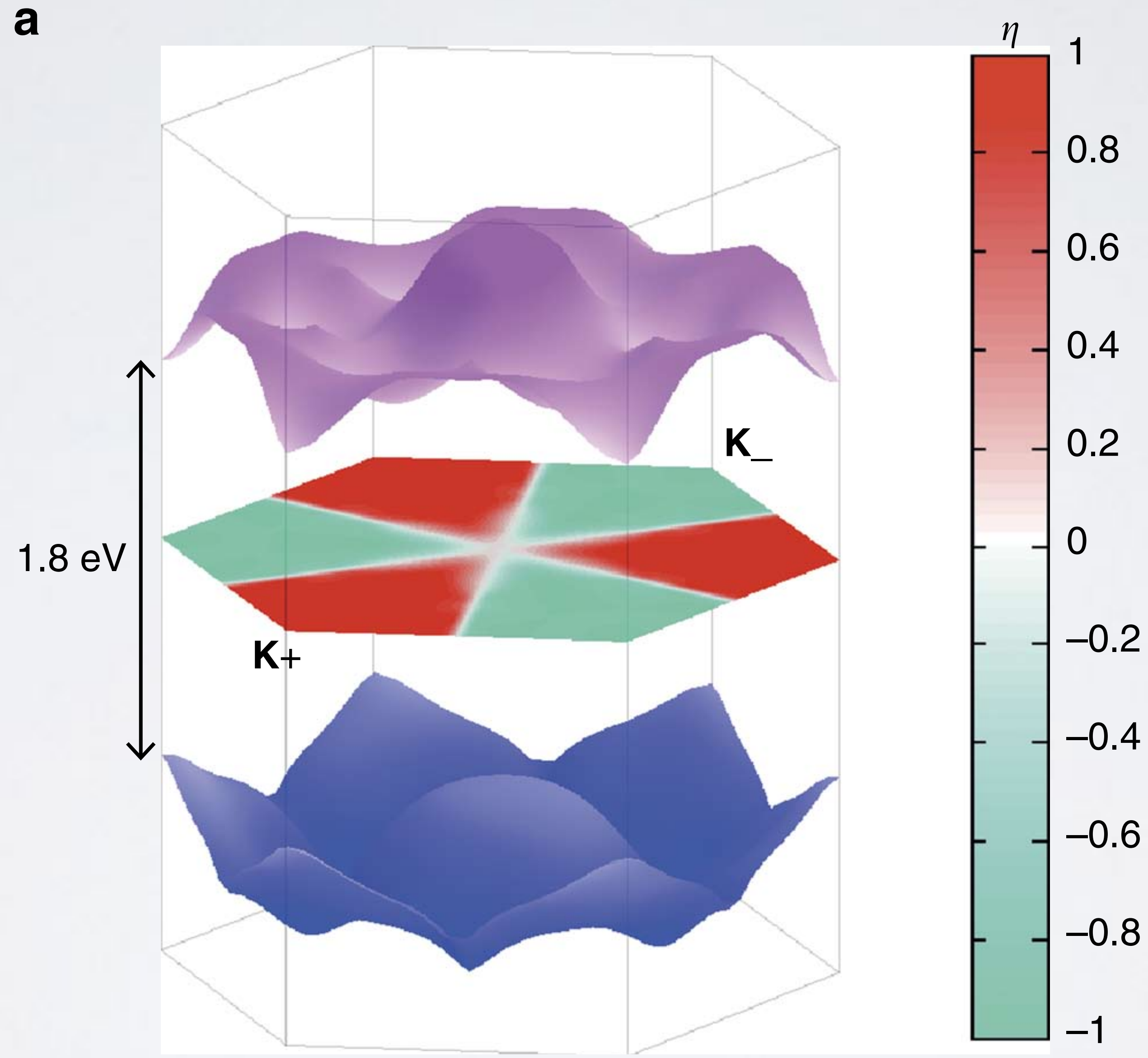
difference between the absorption of left- and right-handed lights, between the top of the valence bands and the bottom of conduction bands

$$\eta(\mathbf{k}, \omega_{cv}) = \frac{|\mathcal{P}_{+}^{cv}(\mathbf{k})|^2 - |\mathcal{P}_{-}^{cv}(\mathbf{k})|^2}{|\mathcal{P}_{+}^{cv}(\mathbf{k})|^2 + |\mathcal{P}_{-}^{cv}(\mathbf{k})|^2}$$

circular polarization: $\mathcal{P}_{\pm}^{cv} = \frac{1}{\sqrt{2}}[P_x^{cv}(\mathbf{k}) \pm i P_y^{cv}(\mathbf{k})]$

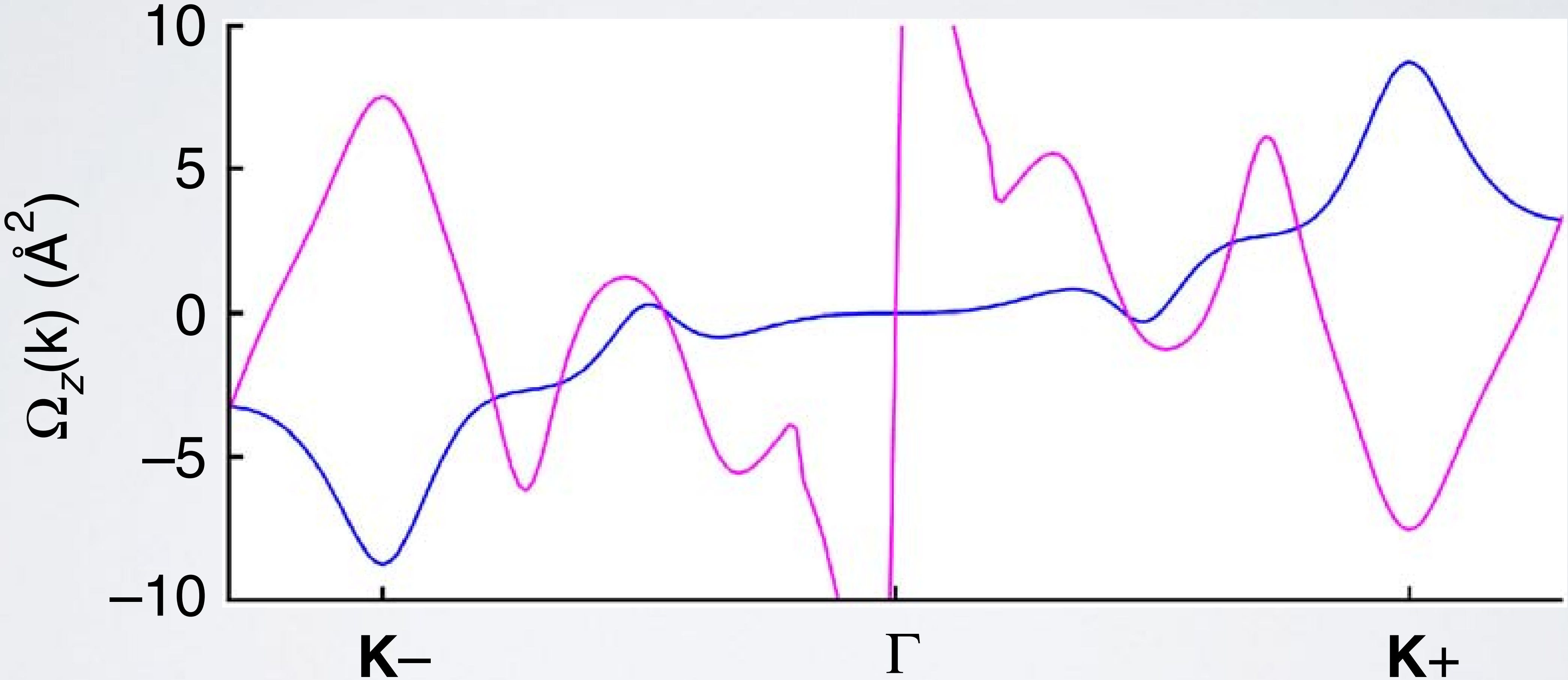
inter-band matrix elements: $\mathbf{P}^{cv}(\mathbf{k}) = \langle \psi_{c\mathbf{k}} | \hat{\mathbf{p}} | \psi_{v\mathbf{k}} \rangle$

η at $K^{\pm}$ in MoS_2

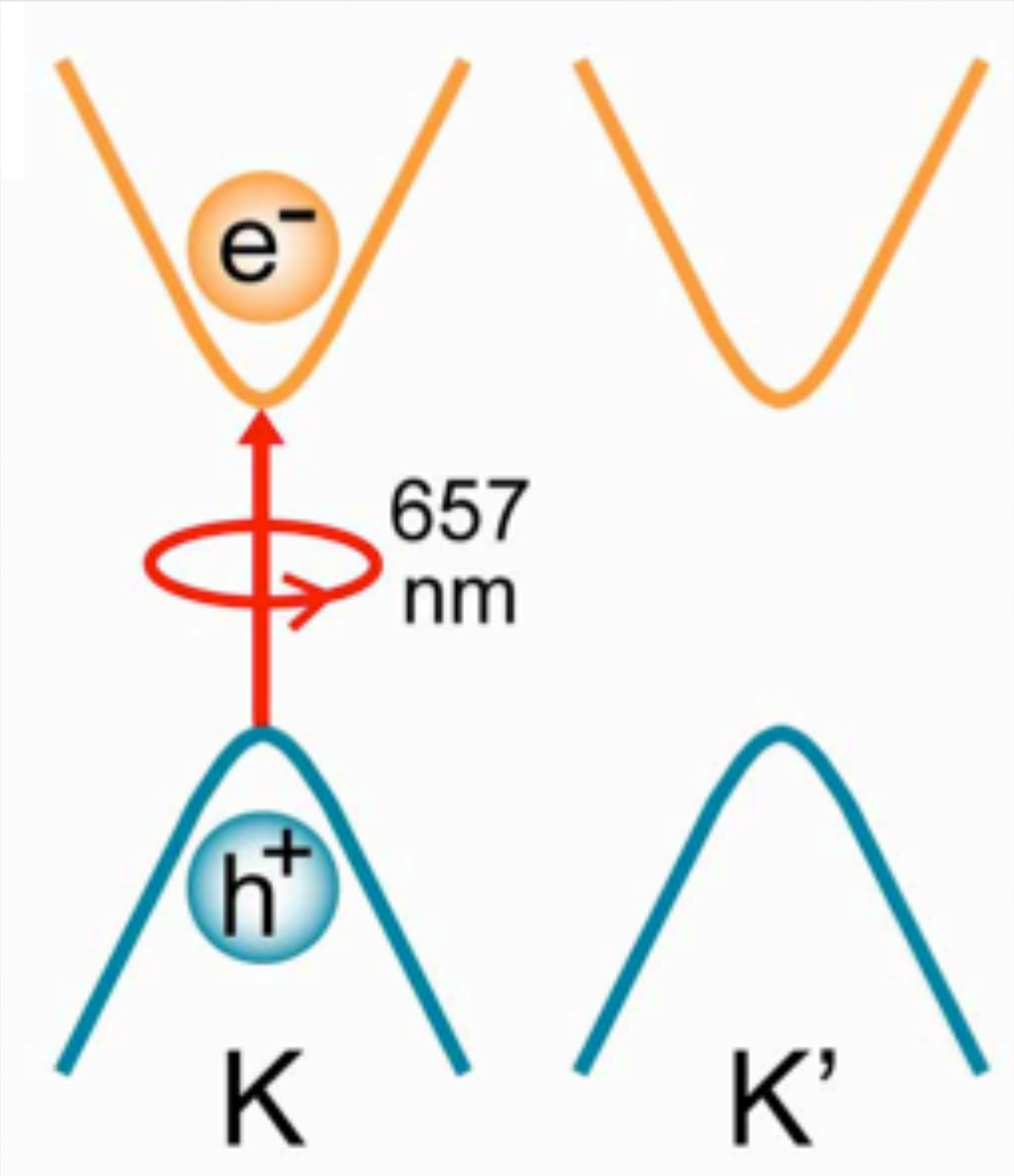


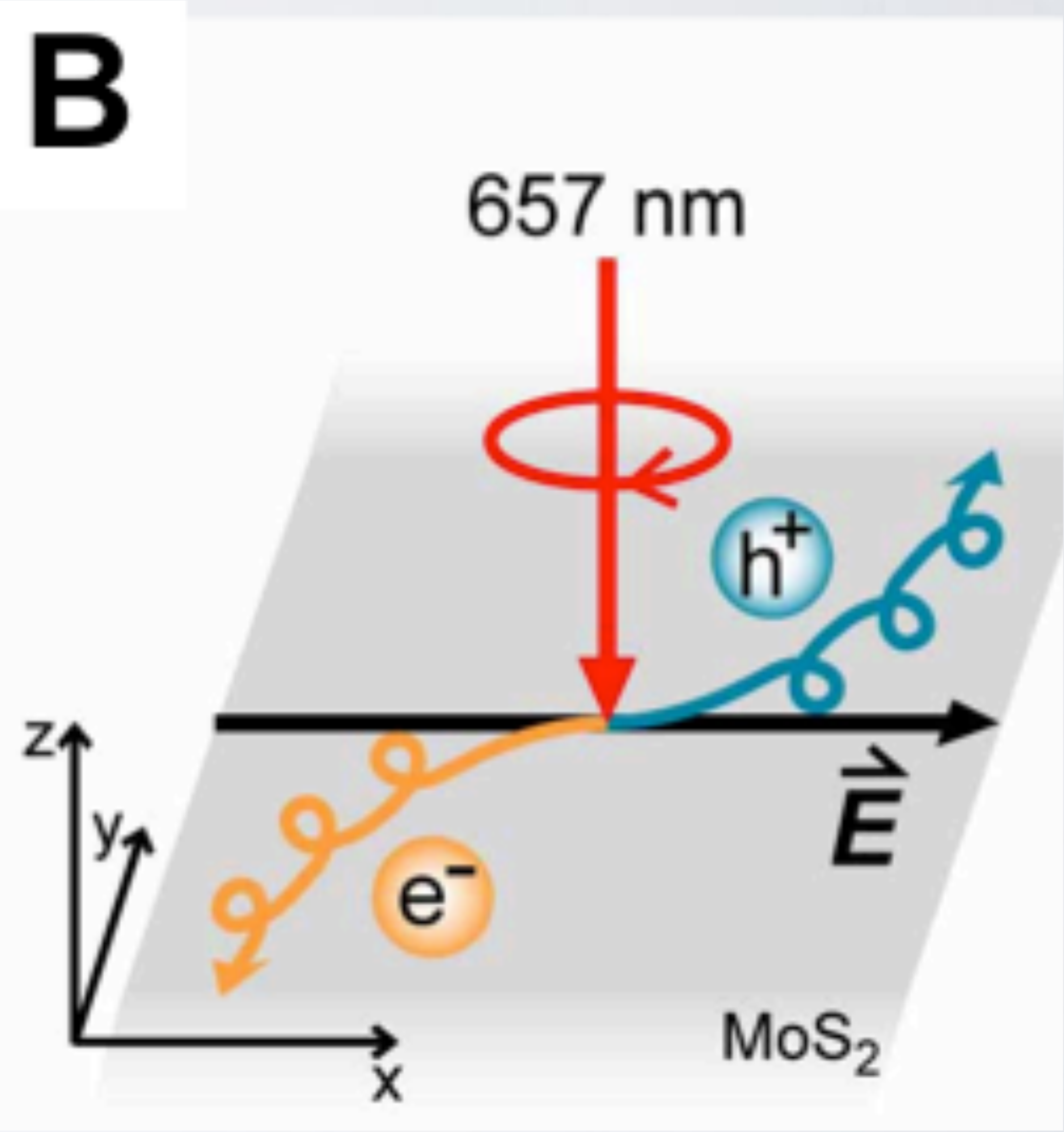
$$\eta(K_+) = +1, \eta(K_-) = -1$$

Berry curvature



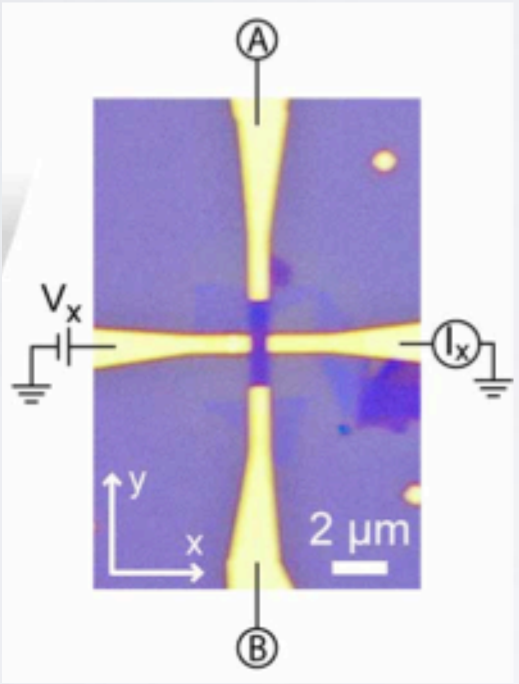
Hall effect

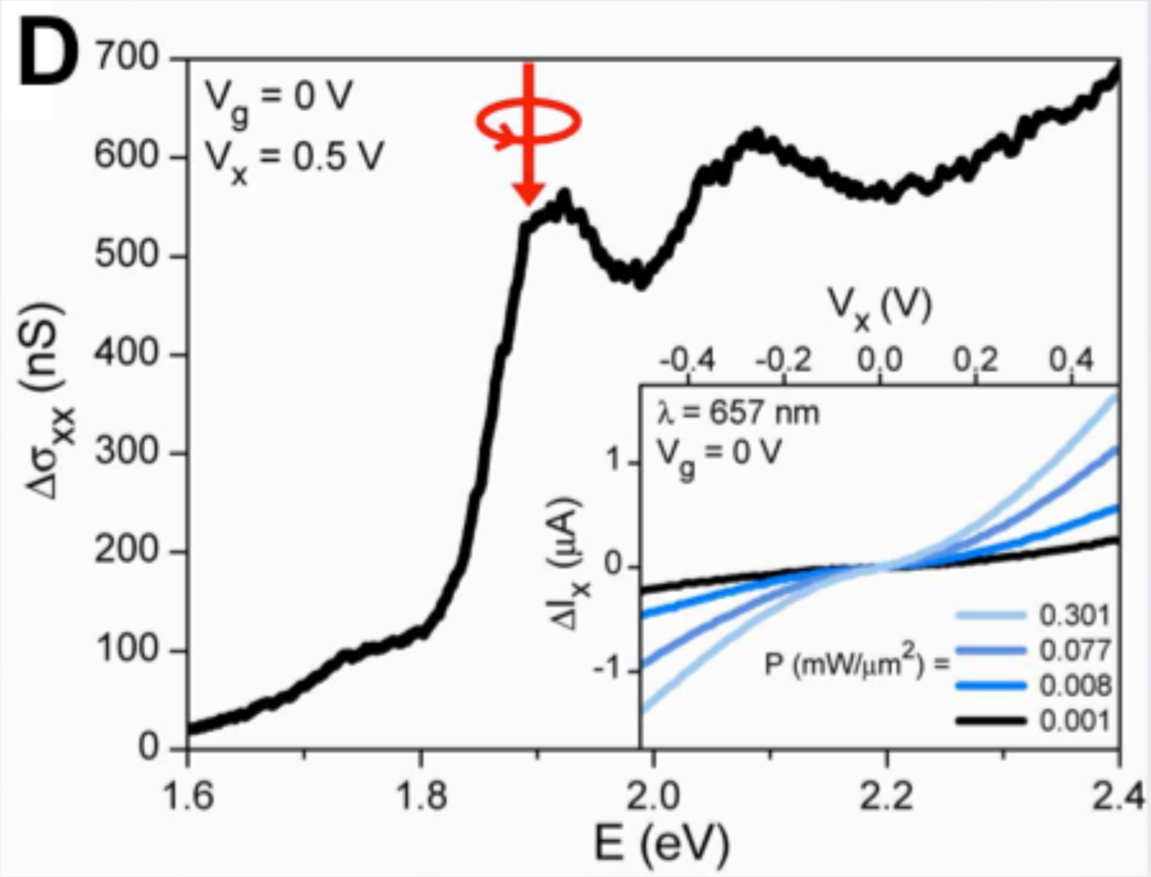




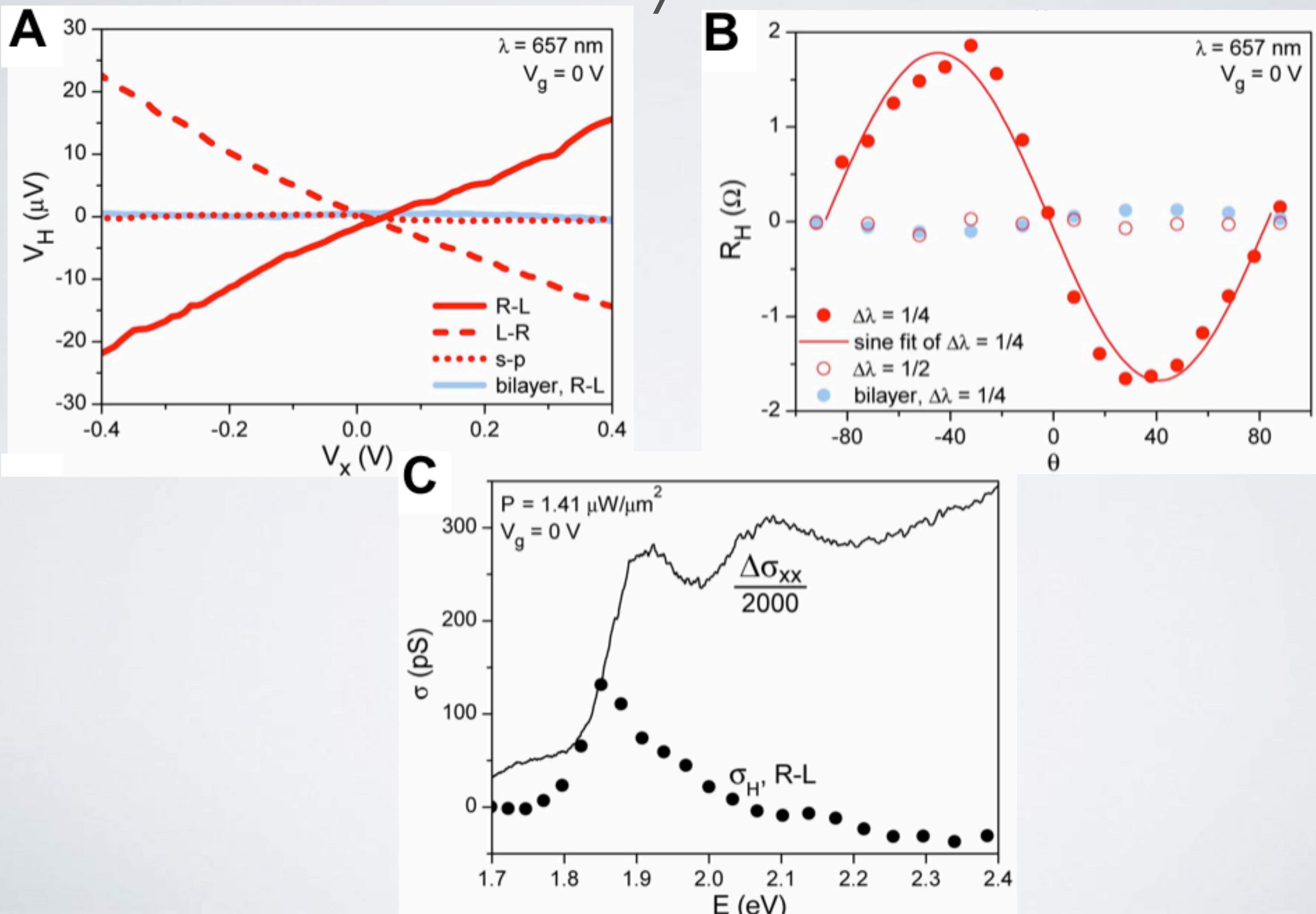
4. The valley Hall effect in MoS_2 transistors

Monolayer MoS_2 Hall bar device

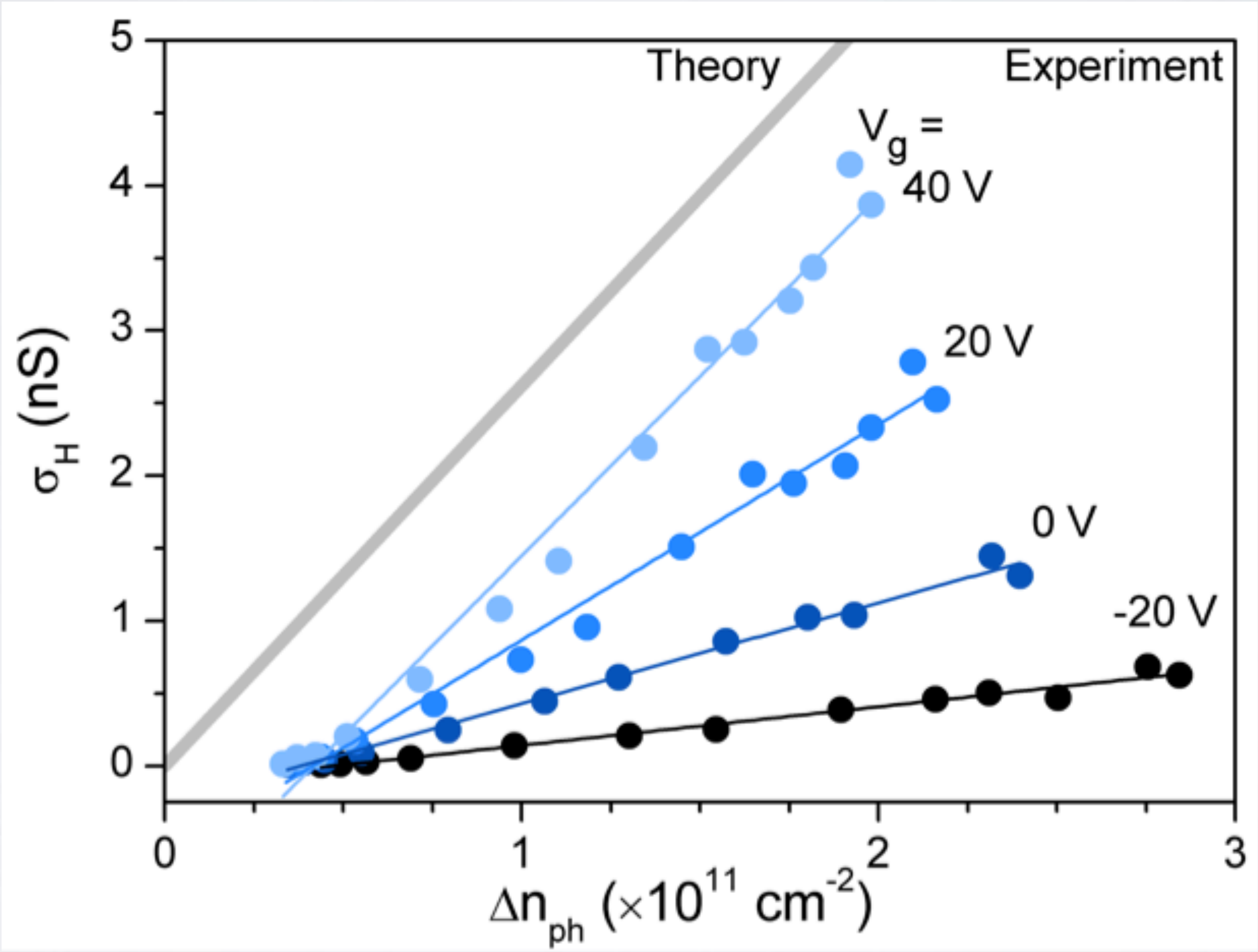




The valley Hall effect



Doping dependence of the anomalous Hall conductivity



Open question

- What does cause the observed quick drop of Hall conductance at laser frequency? Inter-corn scattering?
- What are the relevant sources of scattering present in MoS_2, and what are their relative strengths?
- What are the next steps towards the long standing goal of valleytronics?

Summary

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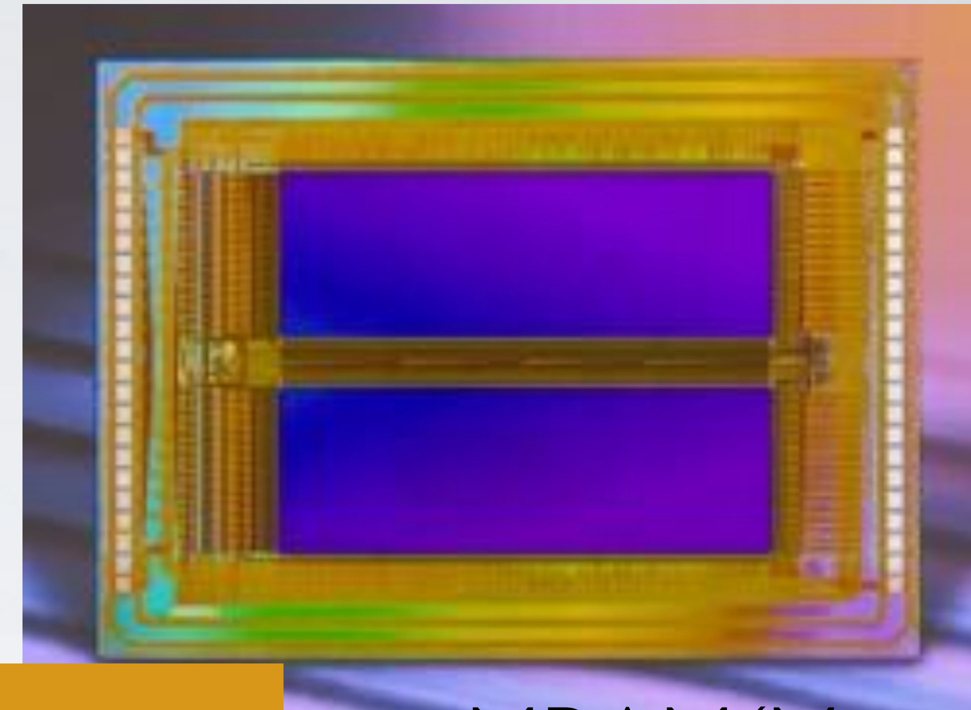
Electronics

Spintronics



MRAM(Motorola)

Valleytronics

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Don’t miss it!