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Optical Hall effect in graphene by strain engineering

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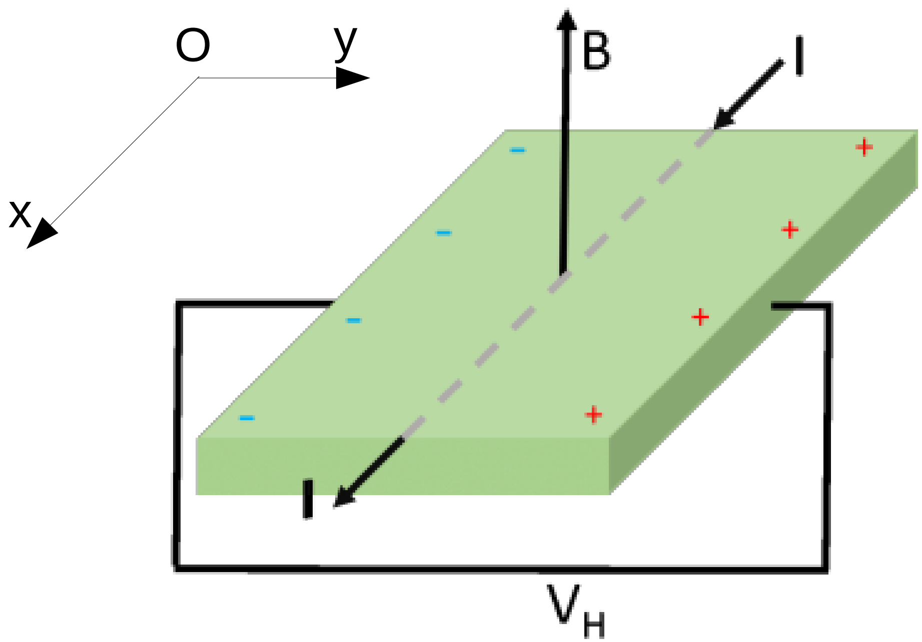
ETSF European Theoretical Spectroscopy Facility

Introduction: Hall effect



Hall current

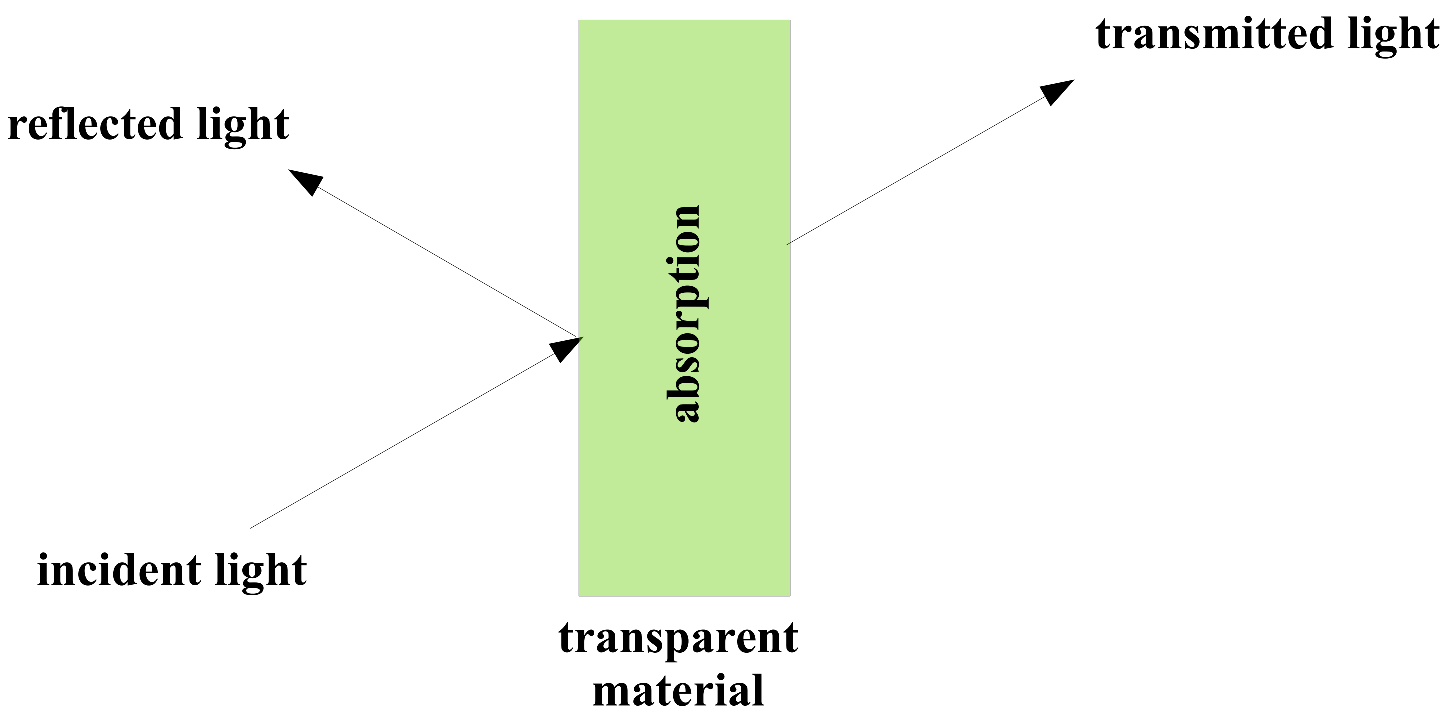
$$J_y = \sigma_H E_x$$

Hall conductivity

Observation of V_H (along Oy) when I (along Ox) and B (along Oz) are applied

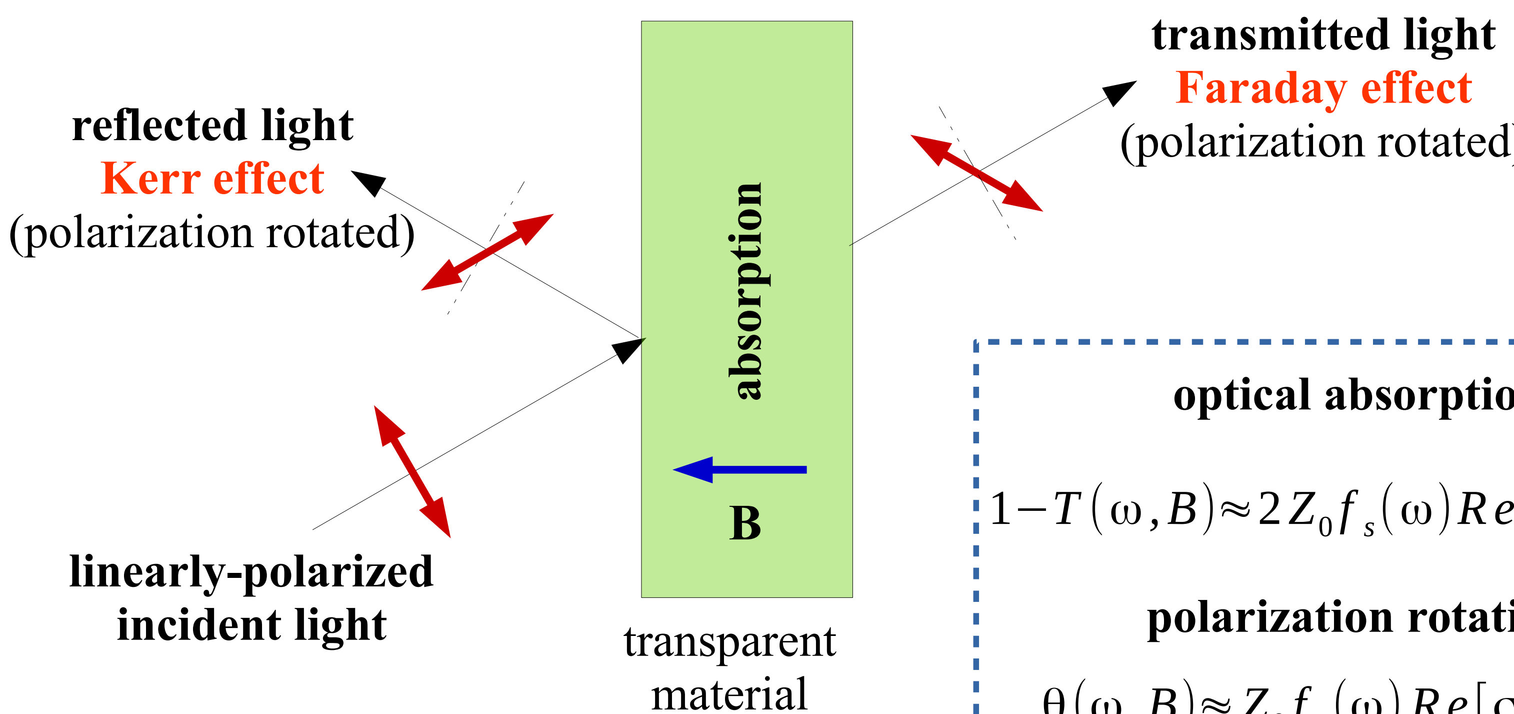
Introduction: optical Hall effect

Interaction between light and charge carriers



Introduction: optical Hall effect

Interaction between light and charge carriers



optical absorption:

$$1 - T(\omega, B) \approx 2 Z_0 f_s(\omega) Re[\sigma_{xx}(\omega, B)]$$

polarization rotation:

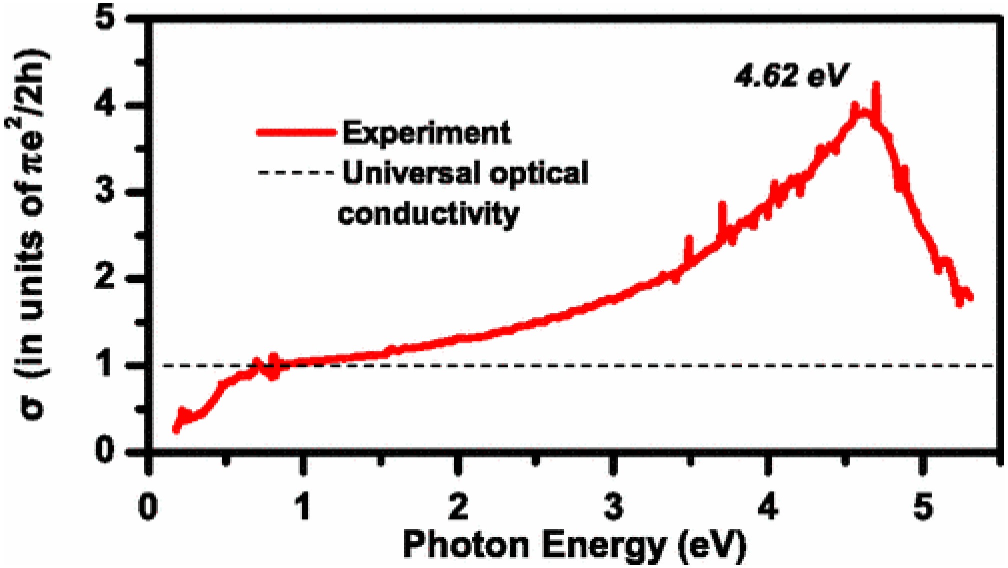
$$\theta(\omega, B) \approx Z_0 f_s(\omega) Re[\sigma_{xy}(\omega, B)]$$

external magnetic field B → optical Hall conductivity $\sigma_{xy}(\omega, B)$

Introduction: optical properties of graphene

Optical spectra:

PRL **106**, 046401 (2011)

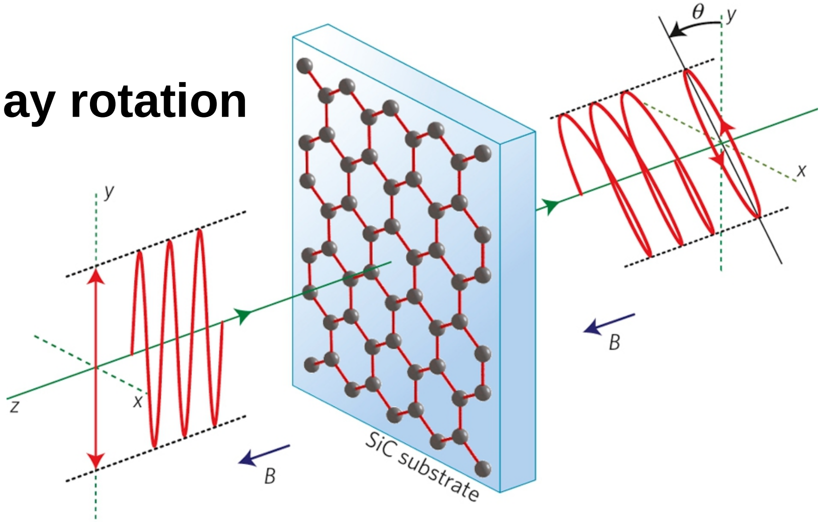


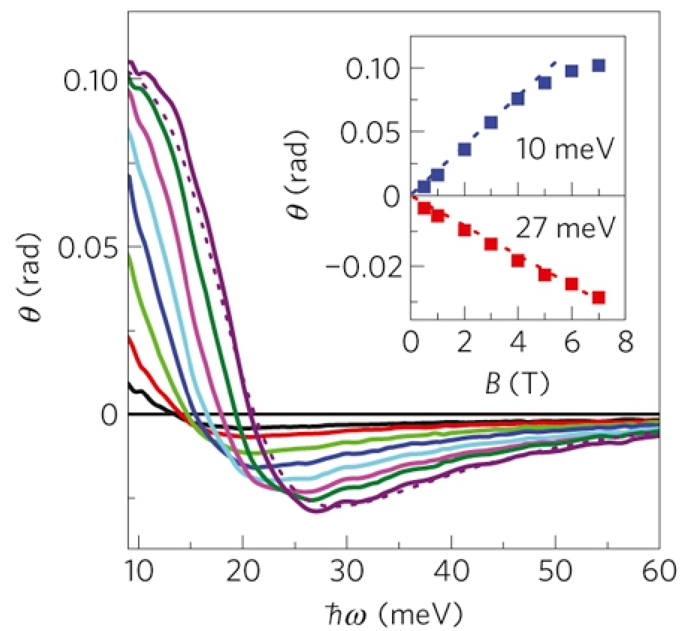
~2.3% absorption

Magneto-optical effects:

Nat. Phys. **7**, 48-51 (2011)

Faraday rotation

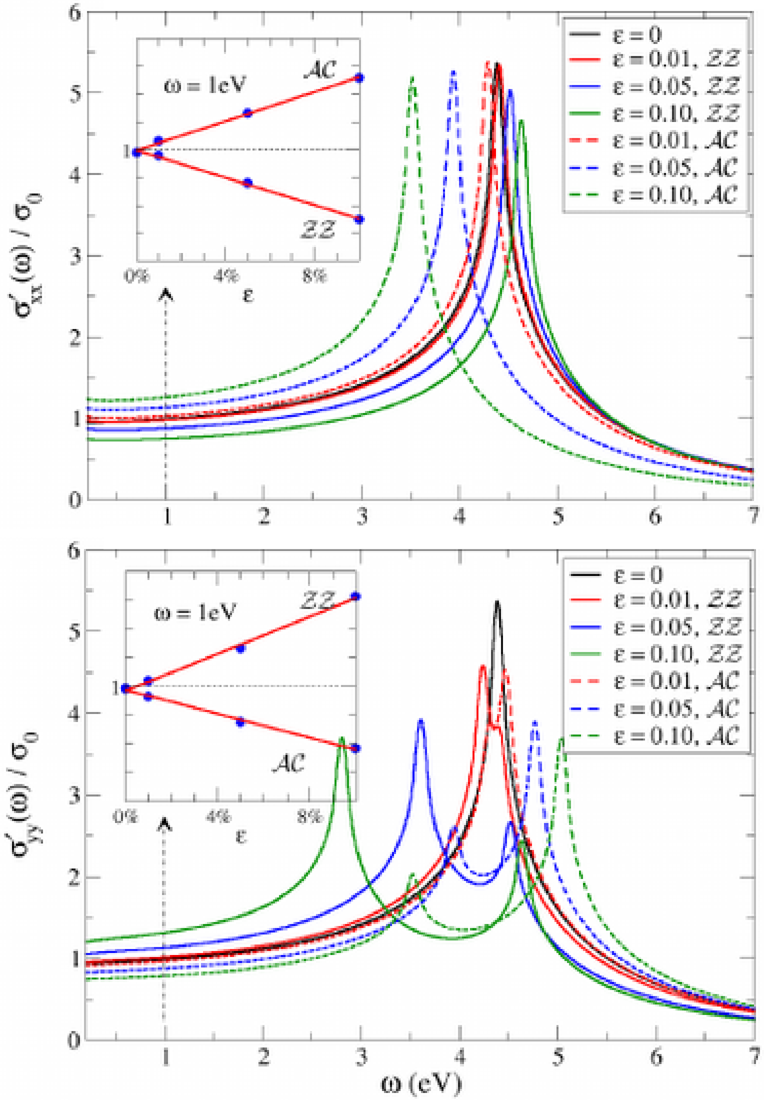




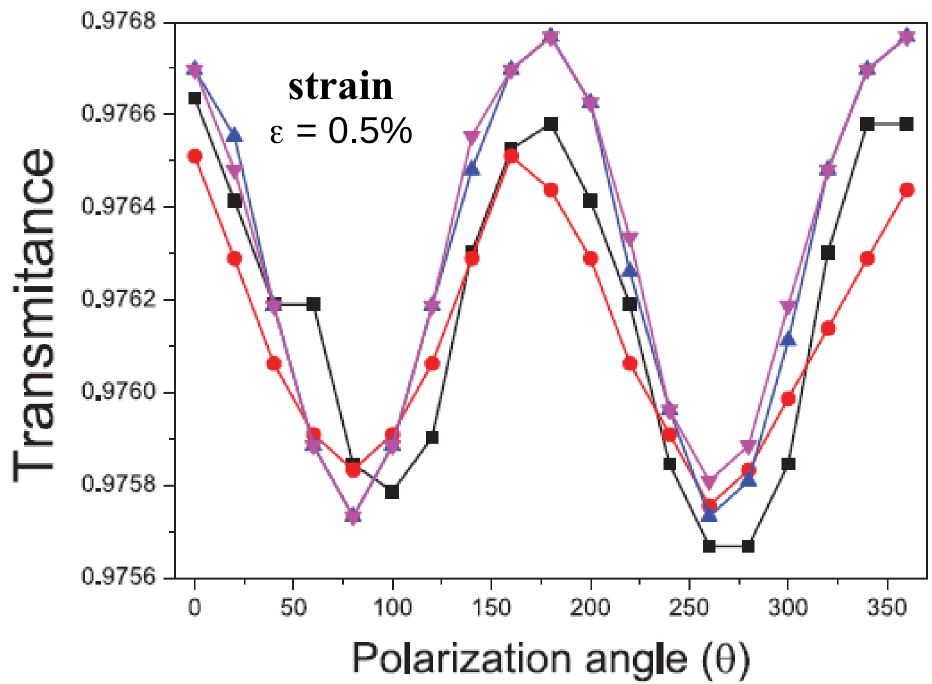
Introduction: optical properties of graphene

Effects of strain:

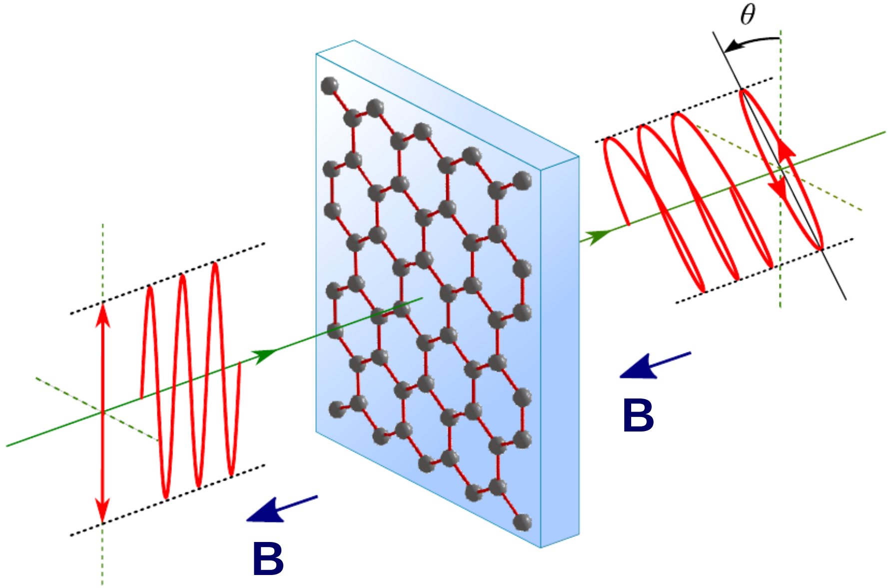
EPL **92**, 67001 (2010): theoretical

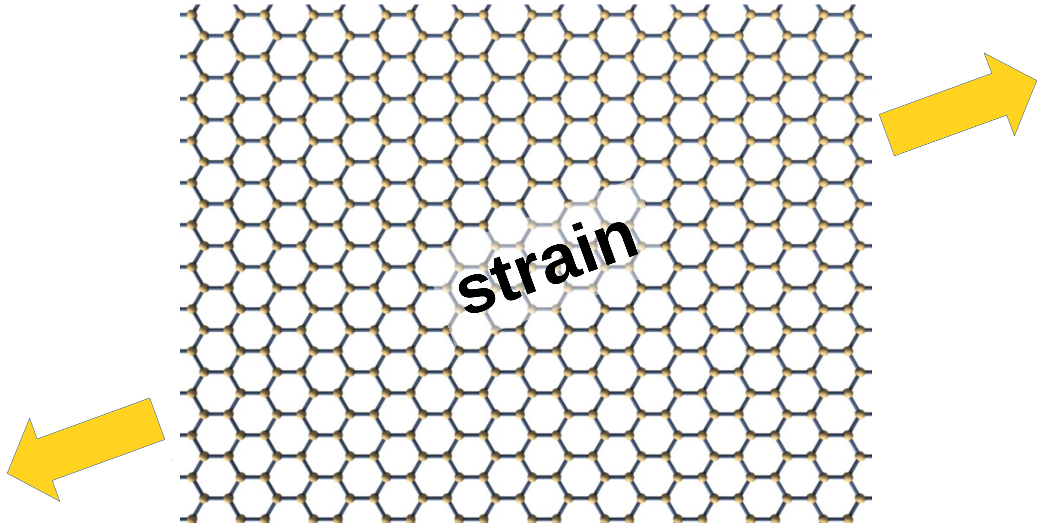


Adv. Mater. **26**, 1081-1086 (2014): experimental



Motivation: optical Hall effect in strained graphene?





B-field:

↓

time reversal symmetry breaking

↓

optical Hall effect

Strain:

↓

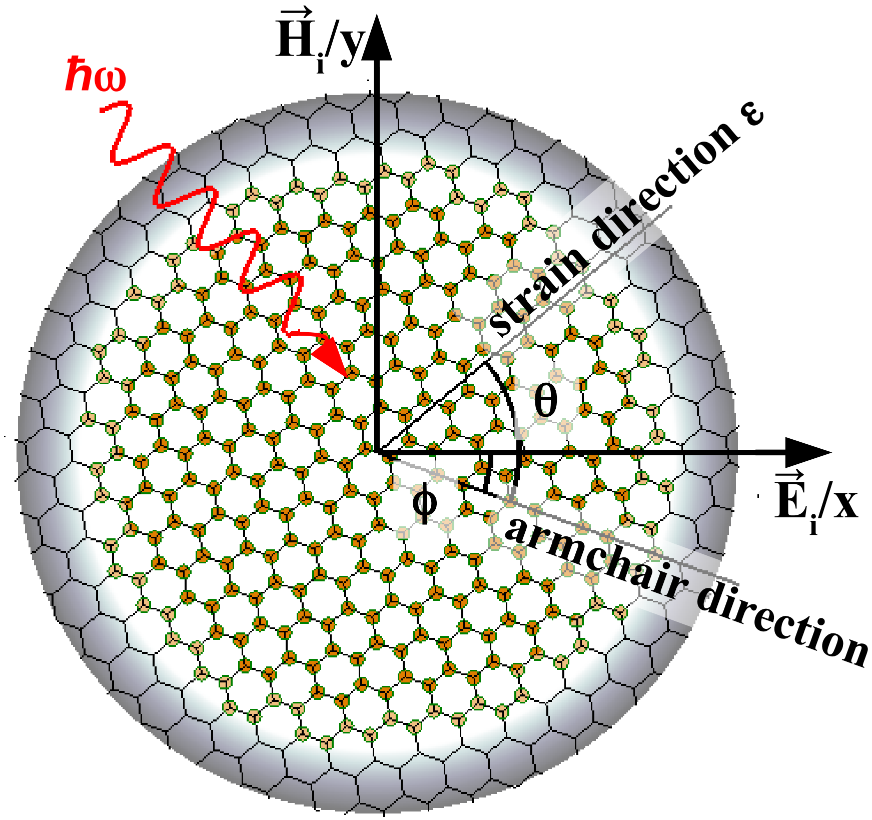
lattice symmetry breaking

↓

zero-field optical Hall effect???

Nguyen *et al.*, 2D Materials **4**, 025041 (2017)

Model and methodologies



- Uniaxial strain: magnitude ε & direction θ
- Light: frequency ω & polarization ϕ

<u>Calculation methods:</u>

- Density functional theory (DFT) with the SIESTA code
- Semi-empirical tight-binding (TB) method with the Kubo formula:

$$\sigma_{pq}(\omega)=\frac{2e^2\hbar}{iS}\sum_{k\in BZ}\sum_{n,m}\frac{f(E_n)-f(E_m)}{E_n(k)-E_m(k)}\frac{\langle n|\hat{v}_p|m\rangle\langle m|\hat{v}_q|n\rangle}{\hbar\omega+E_n(k)-E_m(k)+i\eta}$$

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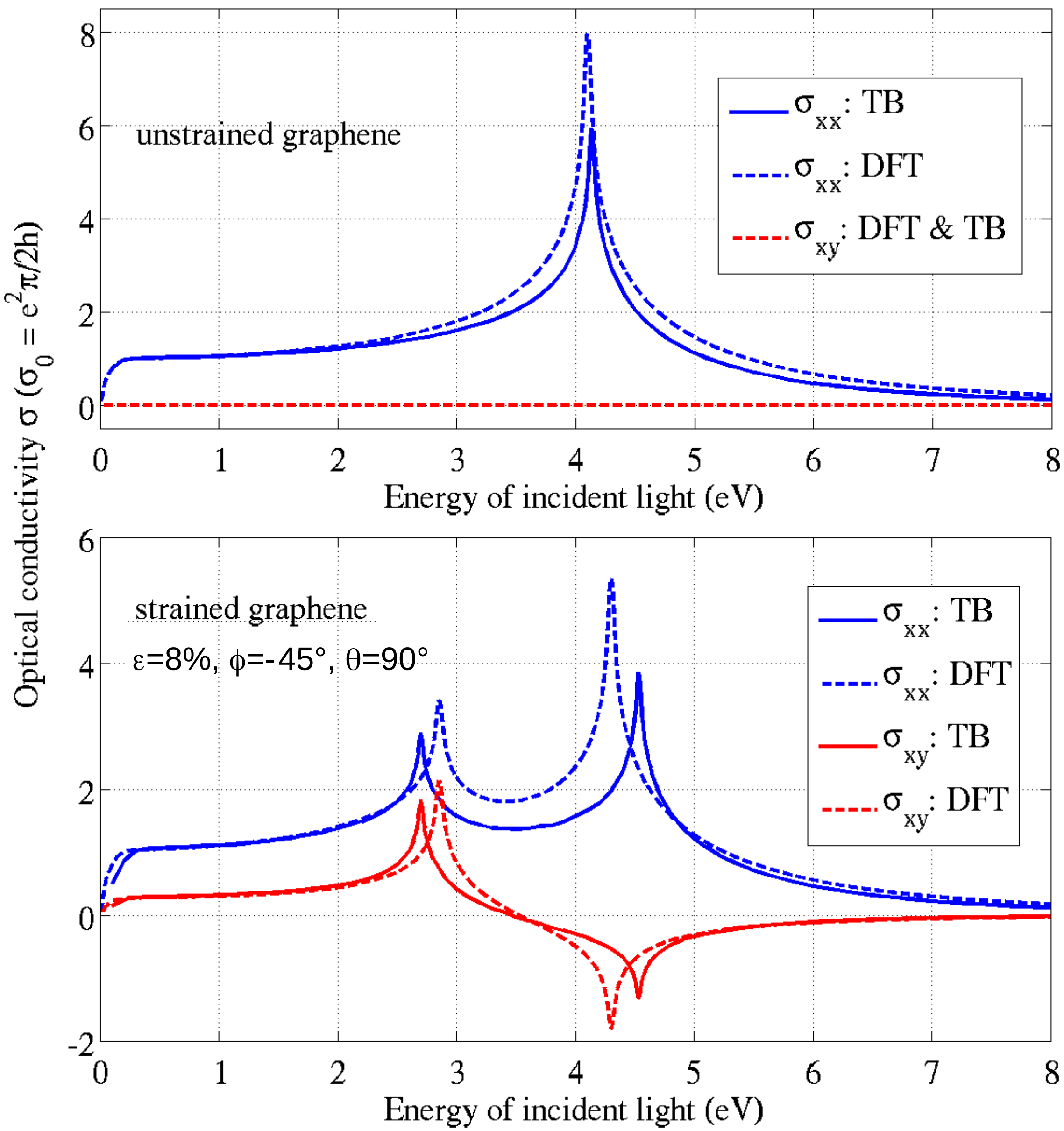
Results: optical Hall conductivity in strained graphene



unstrained graphene:

- zero optical Hall conductivity $\sigma_{xy} = 0$

strained graphene:

- VHS peaks of σ_{xx} are separated

- finite optical Hall conductivity

$\sigma_{xy} > 0$ for low ω

$\sigma_{xy} < 0$ for high ω

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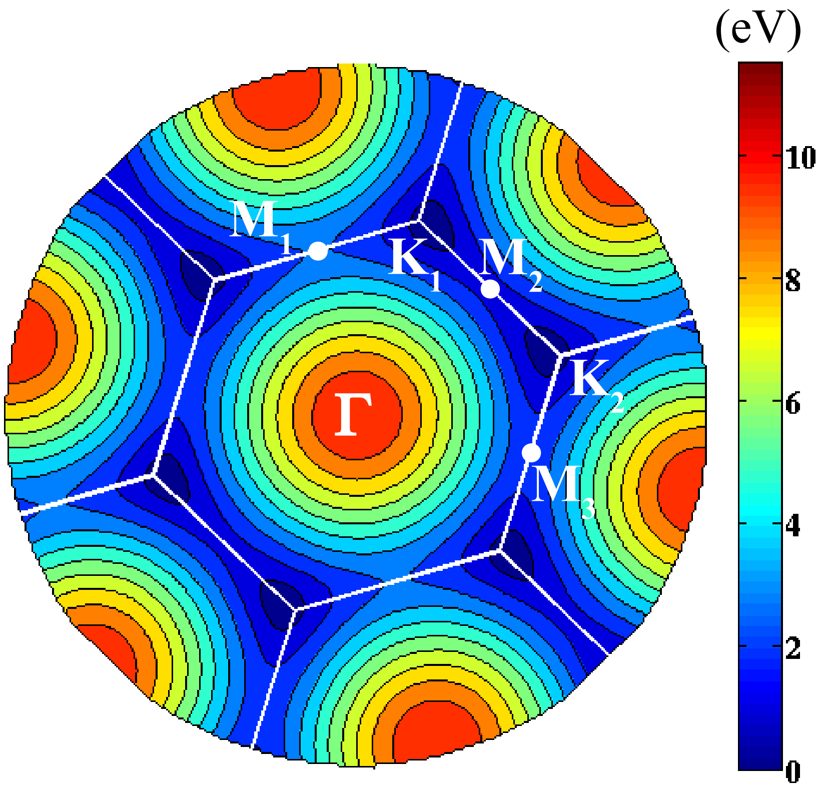
Results: optical Hall conductivity in strained graphene



conduction bands

- 2 distinguishable K-points
- 3 distinguishable M-points

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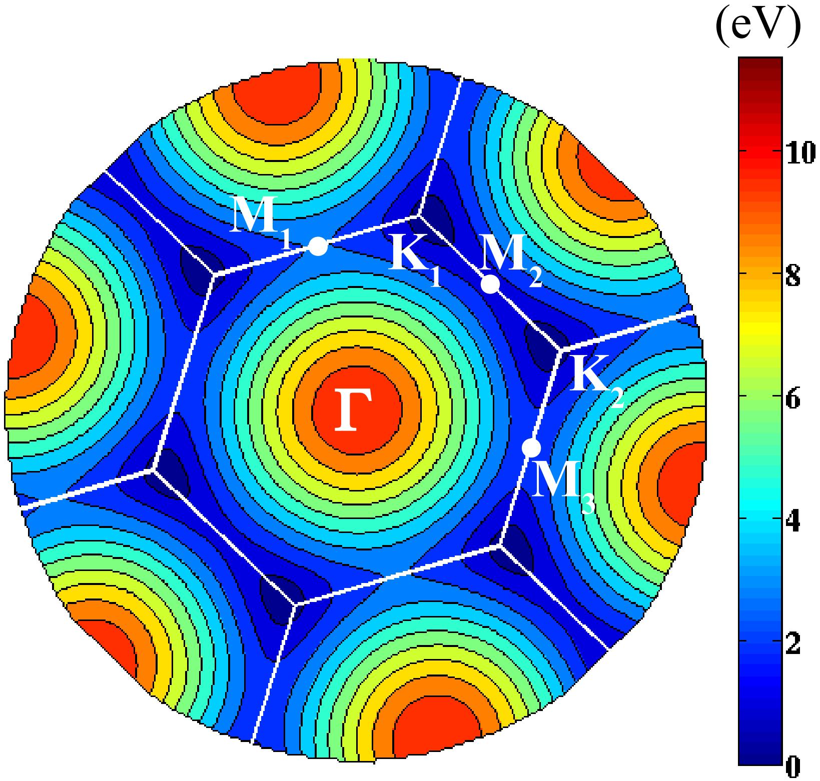
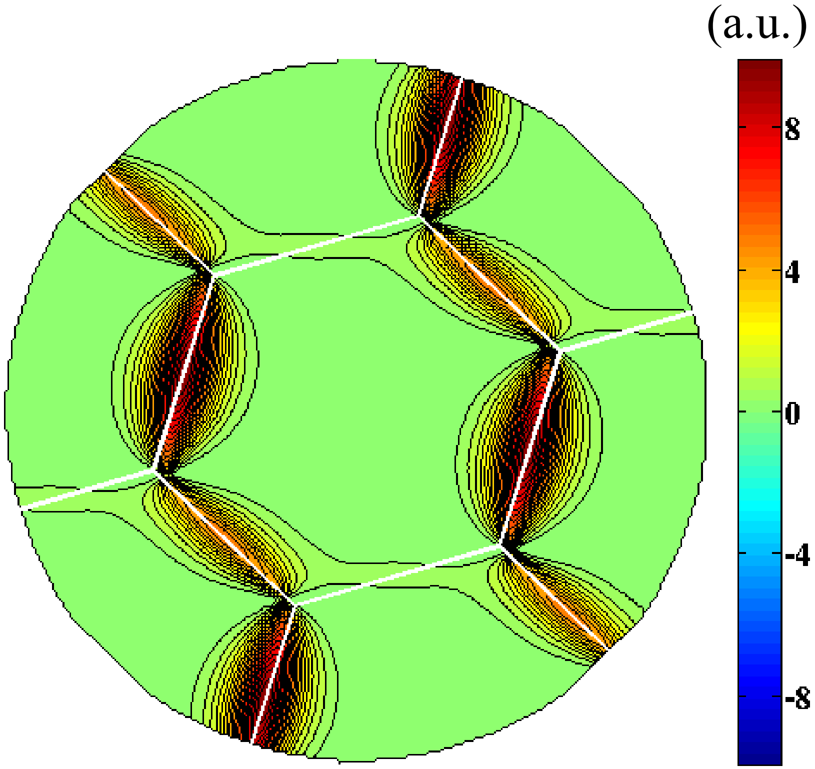
Results: optical Hall conductivity in strained graphene

Kubo formula for optical conductivities

$$\sigma_{pq}(\omega)=\frac{2e^2\hbar}{iS}\sum_{k\in BZ}\sum_{n,m}\cdots\cdots\frac{\langle n|\hat{v}_p|m\rangle\langle m|\hat{v}_q|n\rangle}{\hbar\omega+E_n(k)-E_m(k)+i\eta} \quad \textit{with} \quad C_{pq}(k)=\langle n|\hat{v}_p|m\rangle\langle m|\hat{v}_q|n\rangle$$



conduction bands



coefficient C_{xx}(k)

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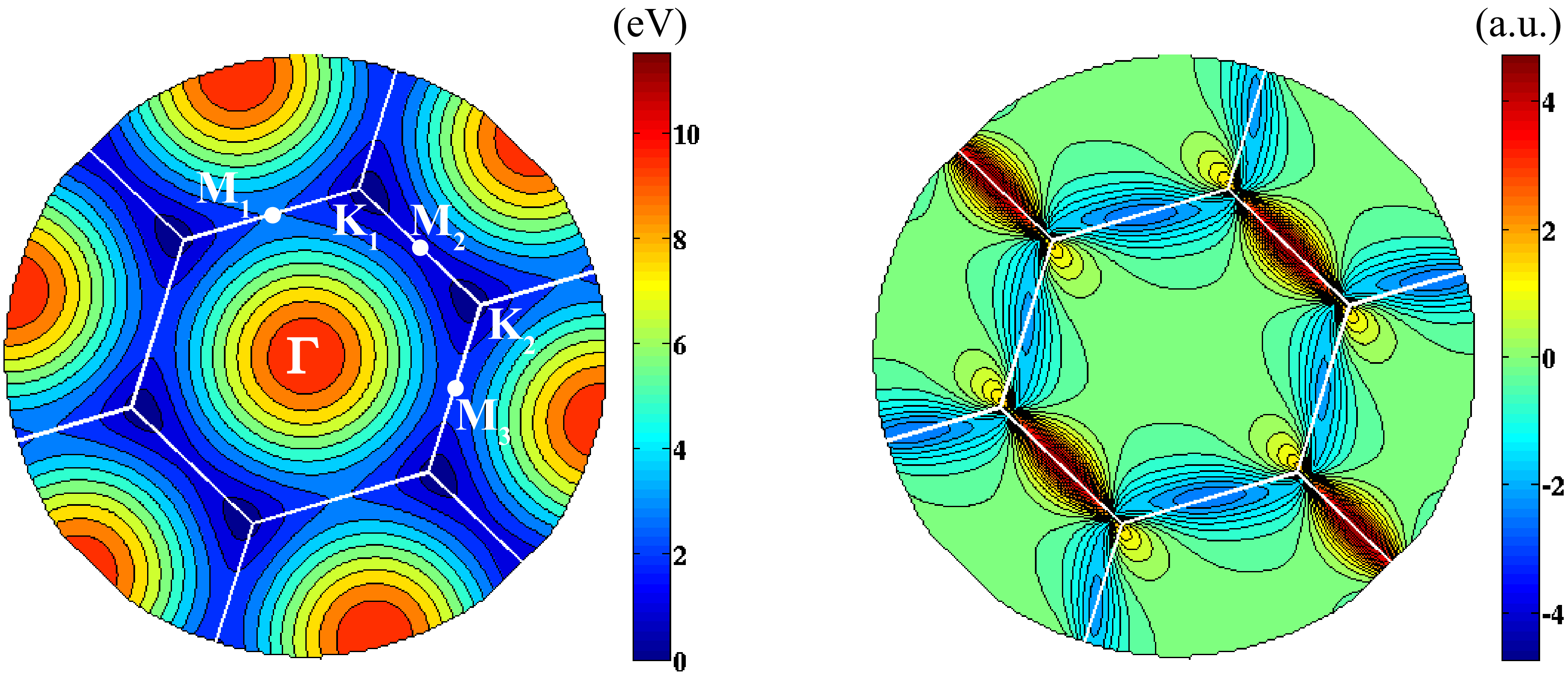
Results: optical Hall conductivity in strained graphene

Kubo formula for optical conductivities

$$\sigma_{pq}(\omega)=\frac{2e^2\hbar}{iS}\sum_{k\in BZ}\sum_{n,m}\cdots\cdots\frac{\langle n|\hat{v}_p|m\rangle\langle m|\hat{v}_q|n\rangle}{\hbar\omega+E_n(k)-E_m(k)+i\eta}\quad with\quad C_{pq}(k)=\langle n|\hat{v}_p|m\rangle\langle m|\hat{v}_q|n\rangle$$



conduction bands

coefficient $C_{xy}(\mathbf{k})$ $\rightarrow$ $\sigma_{xy}=\sigma_{xy}^{+}-\sigma_{xy}^{-}$

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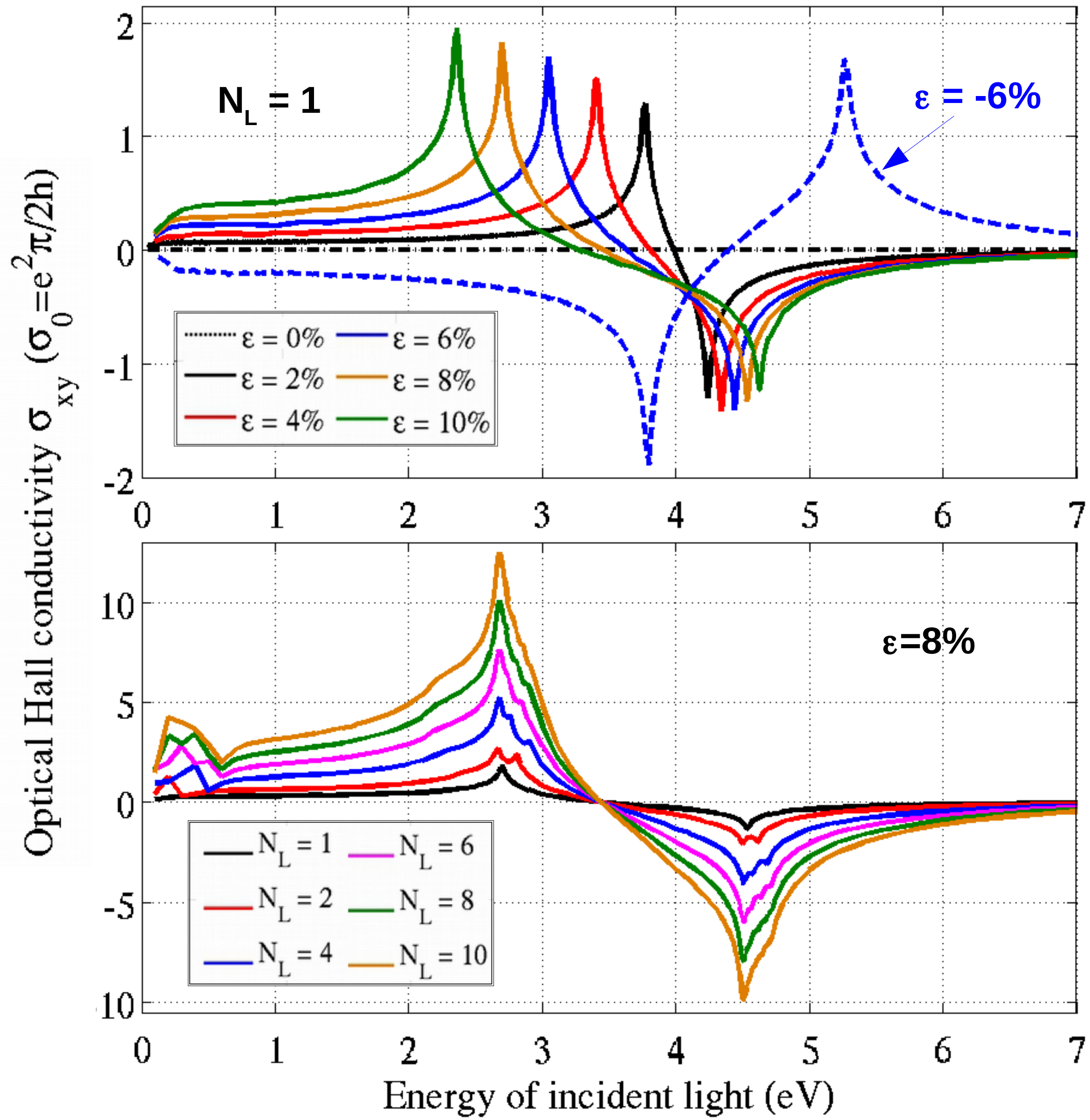
Results: possible large values of σ_{xy}



(1) large values $\sigma_{xy} \sim 1 \div 2\ \sigma_0$ for small strain of ~ a few %

(2) $\sigma_{xy} \propto$ number of layers N_L

(3) sign of σ_{xy} can be reversed by tuning not only ω but also strain type (positive ε or negative ε)

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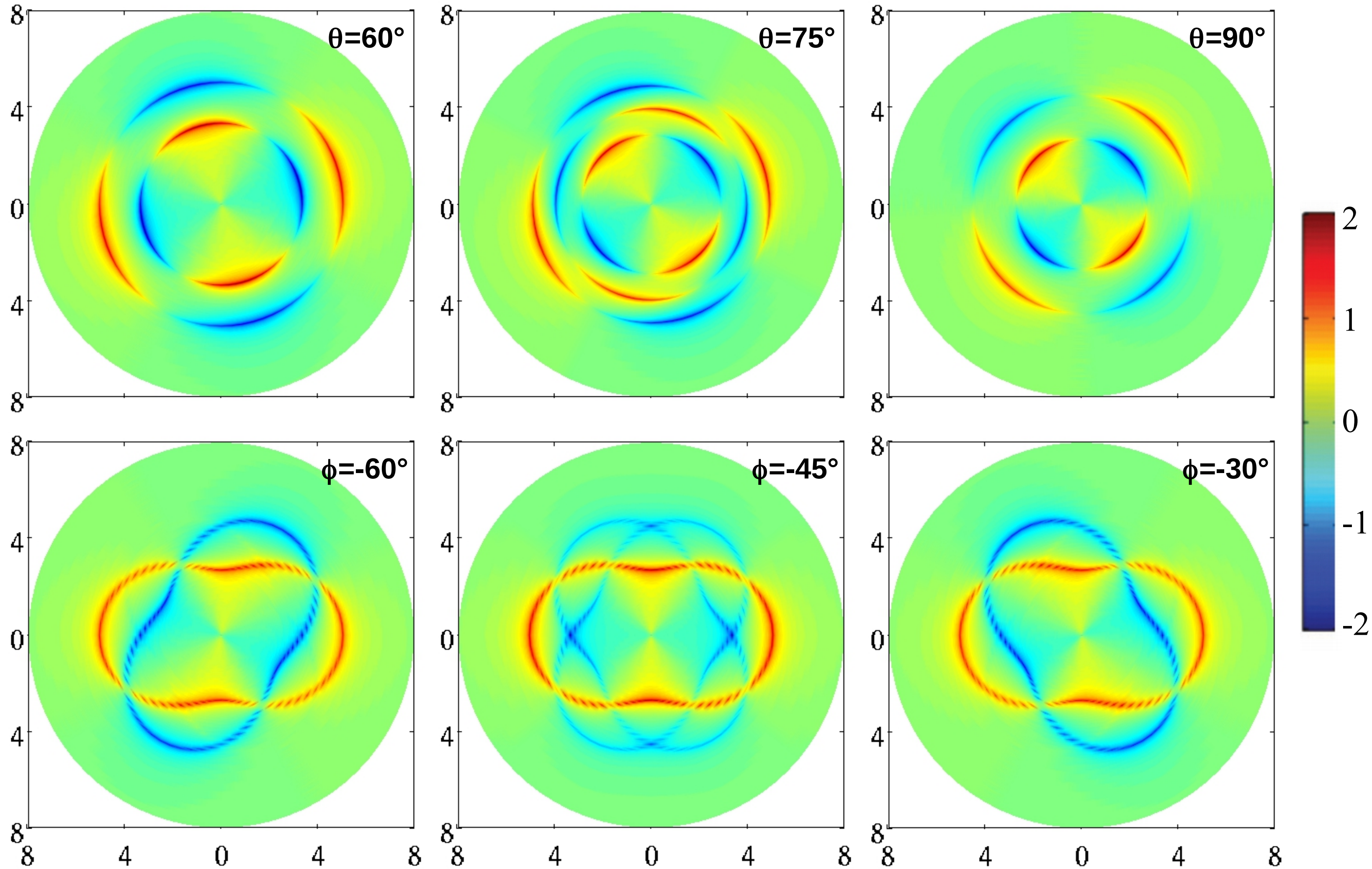
Results: direction dependence of σ_{xy}

ε=8%

(ω,ϕ)-maps →

(ω,θ)-maps →



- σ_{xy} depends only on ω and ε but also light polarization ϕ and strain direction θ
- σ_{xy} generally exhibits three peaks but only two if ϕ or θ ≡ armchair/zigzag direction

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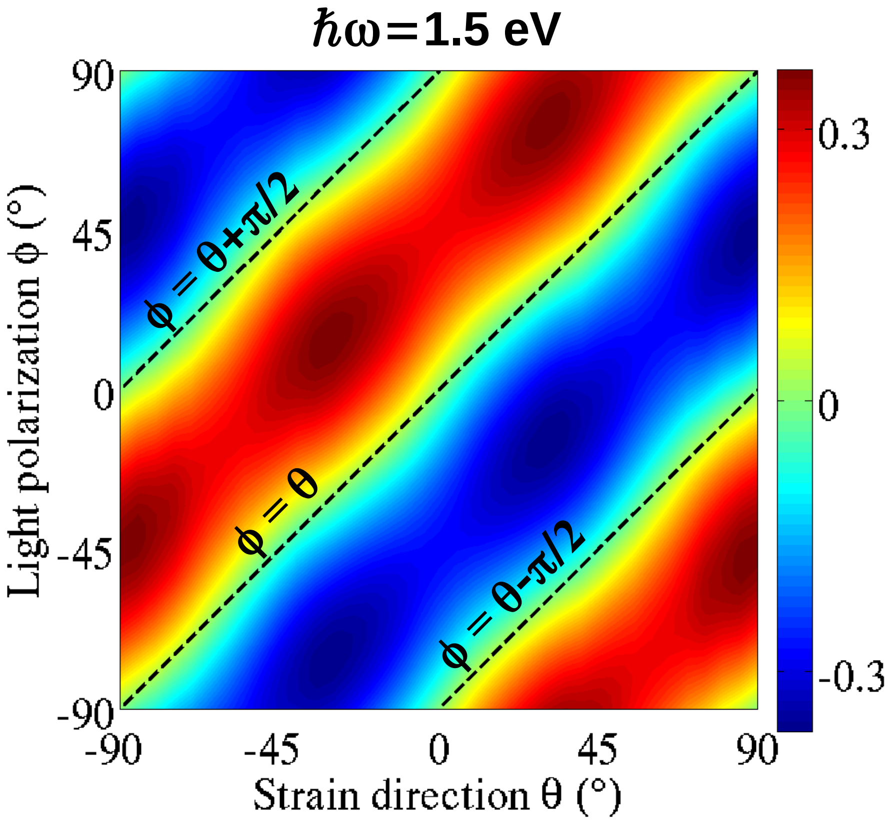
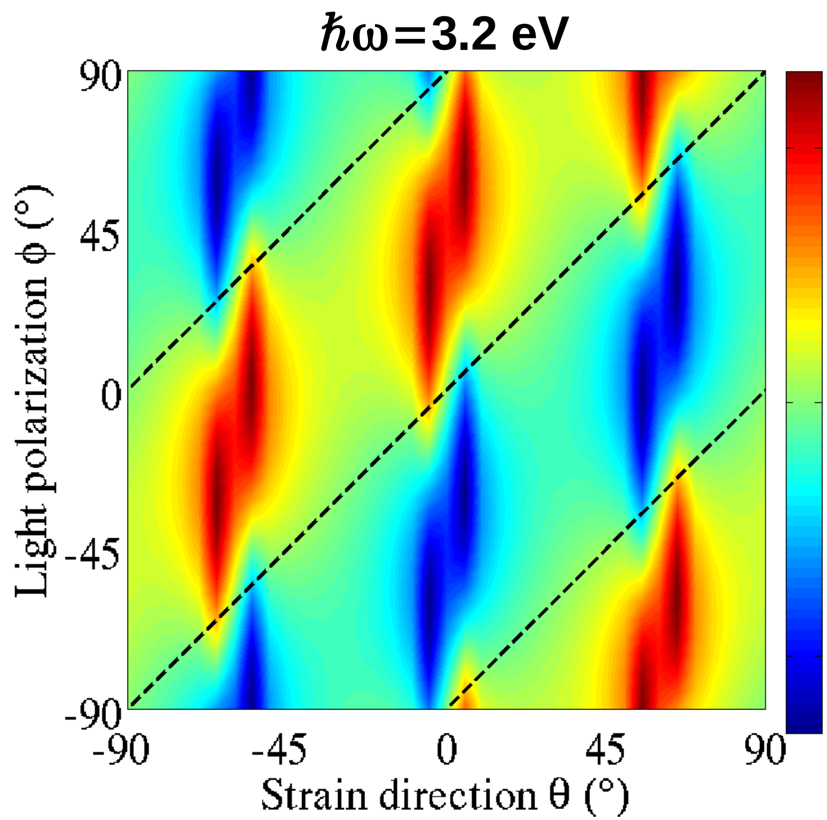
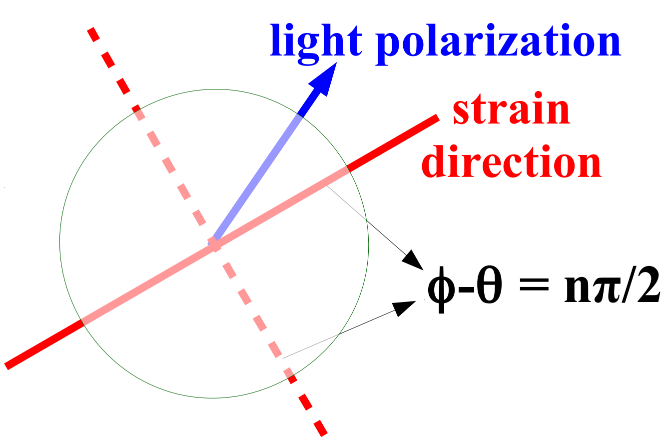
Results: direction dependence of σ_{xy}





$\sigma_{xy} \propto \sin(2(\phi-\theta))$, i.e., small if $\phi-\theta \approx n\pi/2$

and have peaks when $\phi-\theta \approx n\pi/2+\pi/4$



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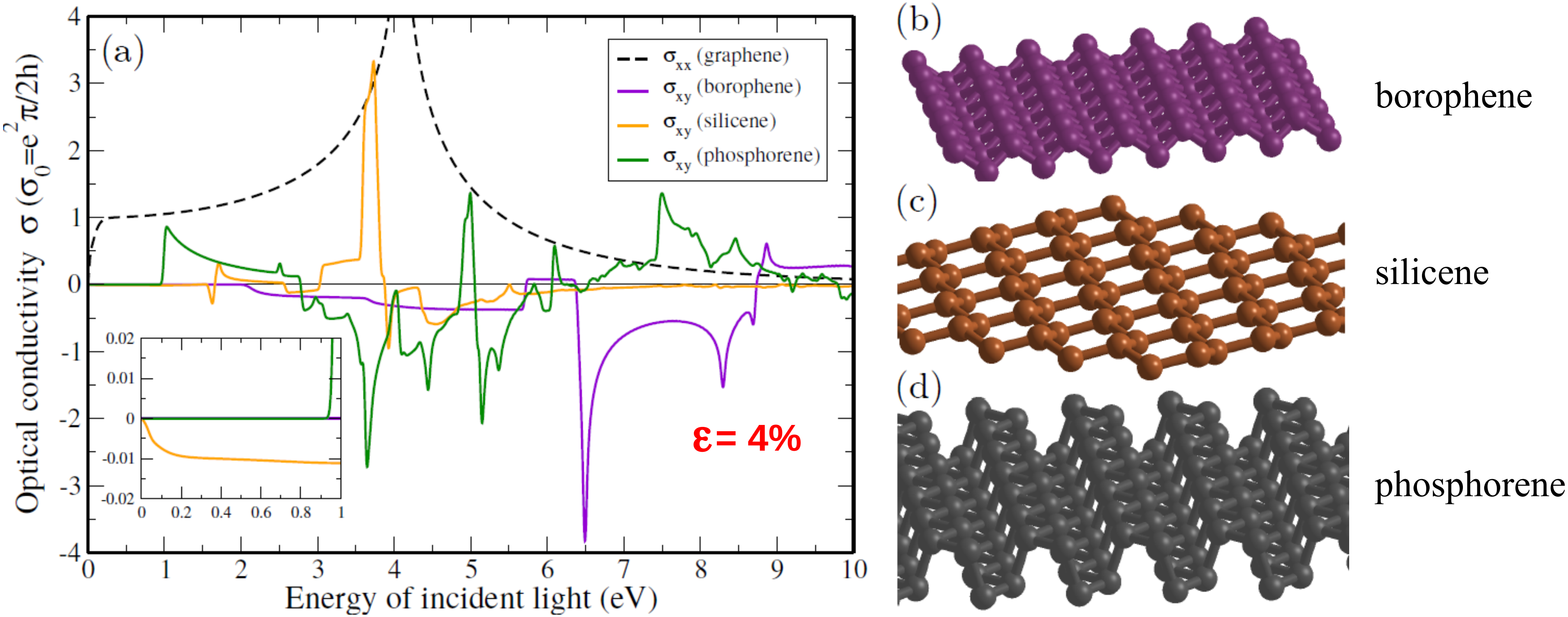
Results: optical Hall effect in other materials



strain engineering: a common technique to generate optical Hall effect!!!

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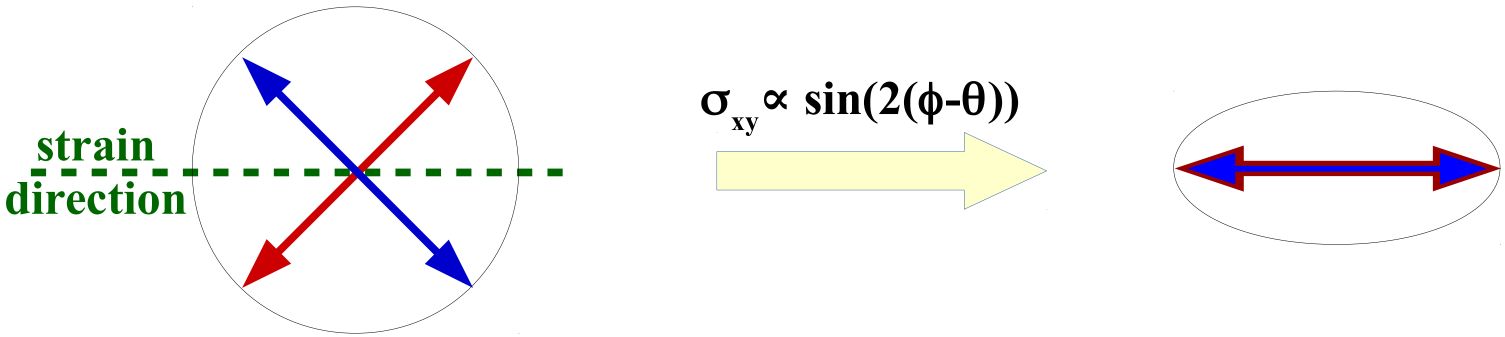
Conclusion

- strain engineering: general/alternative approach to achieve optical Hall effect
- both value and sign of σ_{xy} are tunable by strain (ε,θ) and incident light (ω,ϕ)

=> possible opto-electro-mechanical applications:

e.g., AC Hall systems, optical modulators, sensors, rotators, polarizers?



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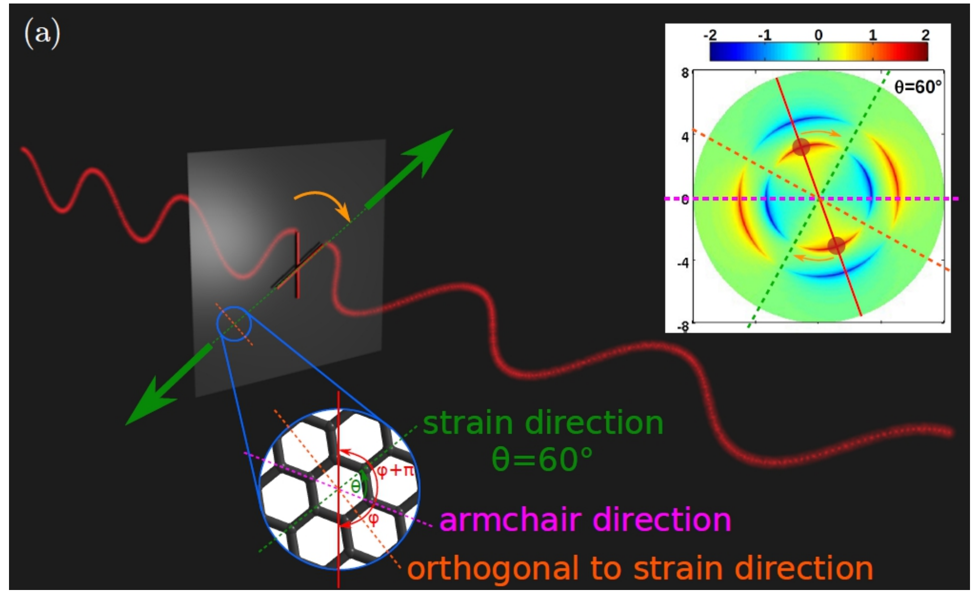
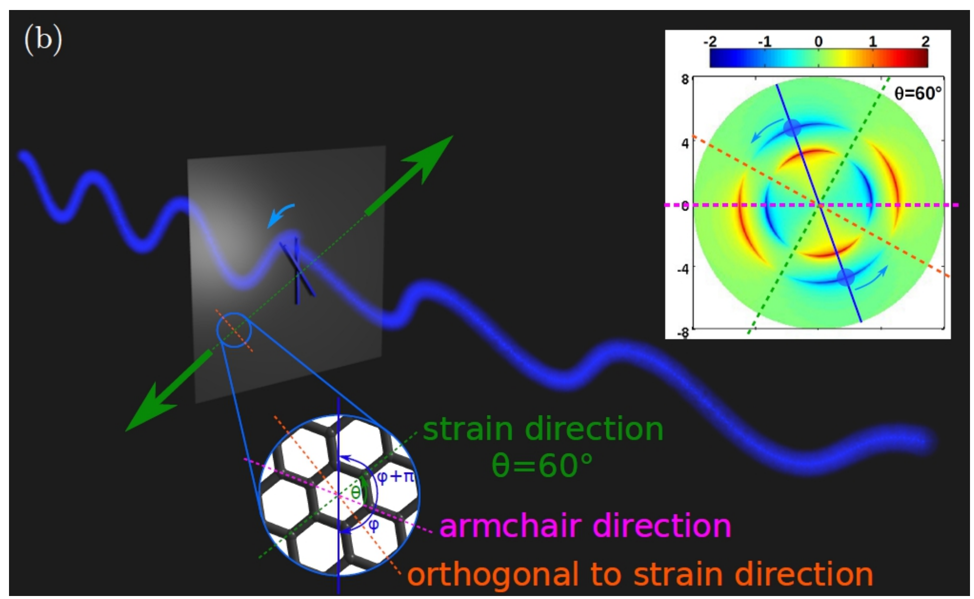
Conclusion

Faraday rotation

- Low energy lights



- High energy lights



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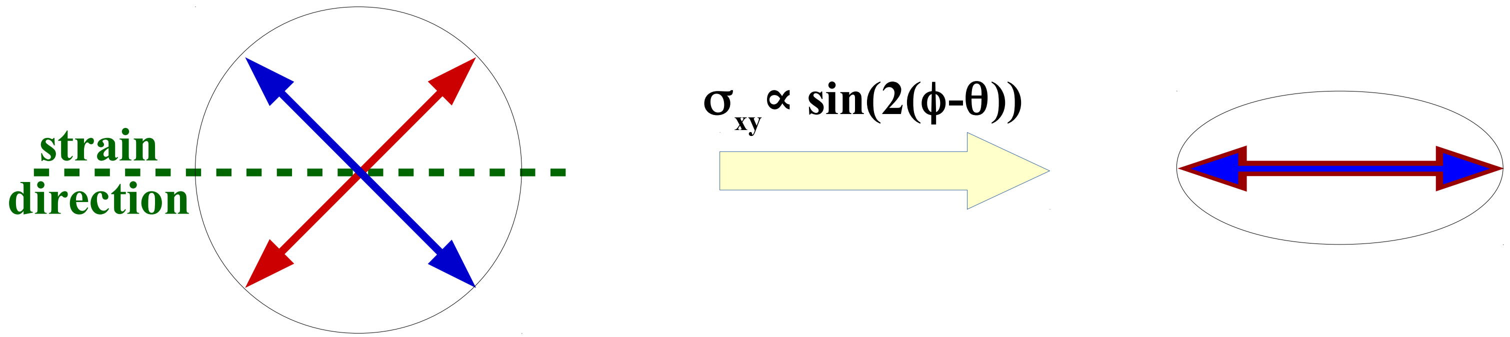

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