New Perspectives in Spintronic and
Mesoscopic Physics (NPSMP2015),
ISSP, Kashiwa, June 17, 2015

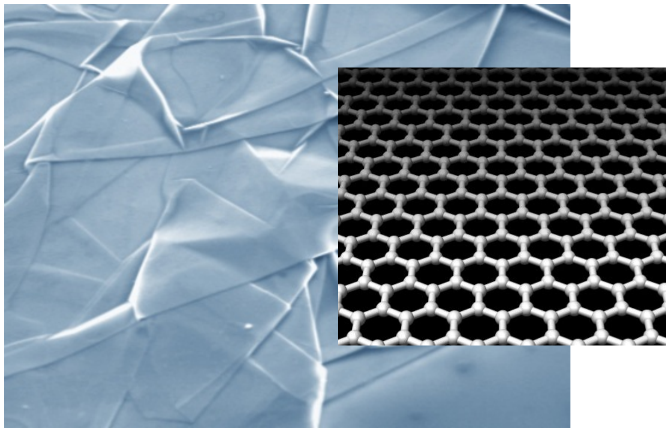
Electronic transmission through the atomic domain boundary

--- from graphene to transition metal dichalcogenides

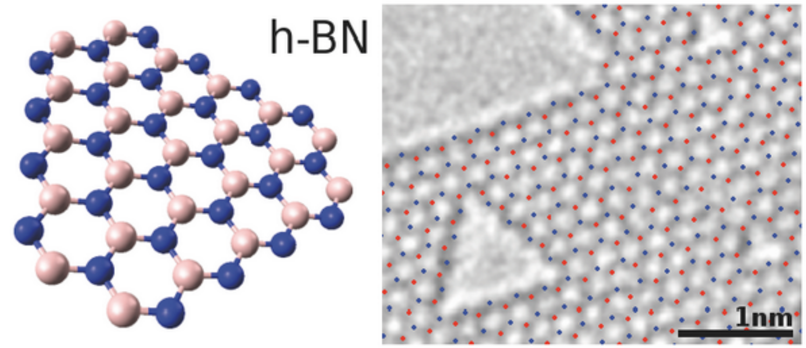
Mikito Koshino (Tohoku University)

Family of 2D materials

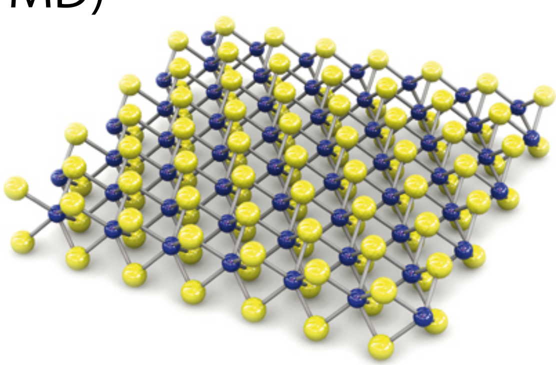
Graphene



hexagonal BN



Transition metal dichalcogenides (TMD)



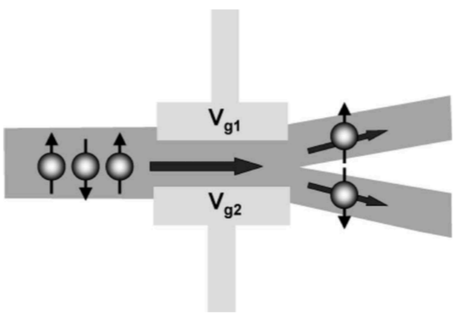
MX_2 (M=Mo,W; X=S, Se,Te)

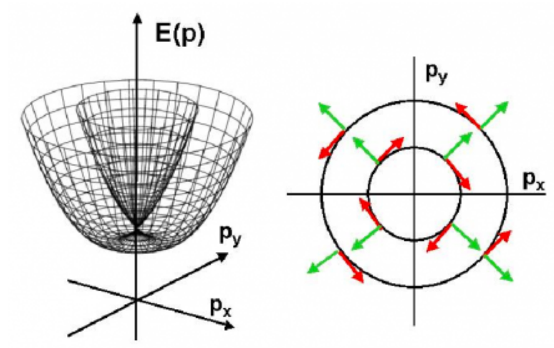
Phosphorene

Nature Nanotechnology 9, 330–331 (2014) DOI: 10.1038/nnano.2014.85

Spintronics in 2D materials?

Ex. Spin splitters proposed in conventional 2DEG (Rashba spin-orbit interaction)





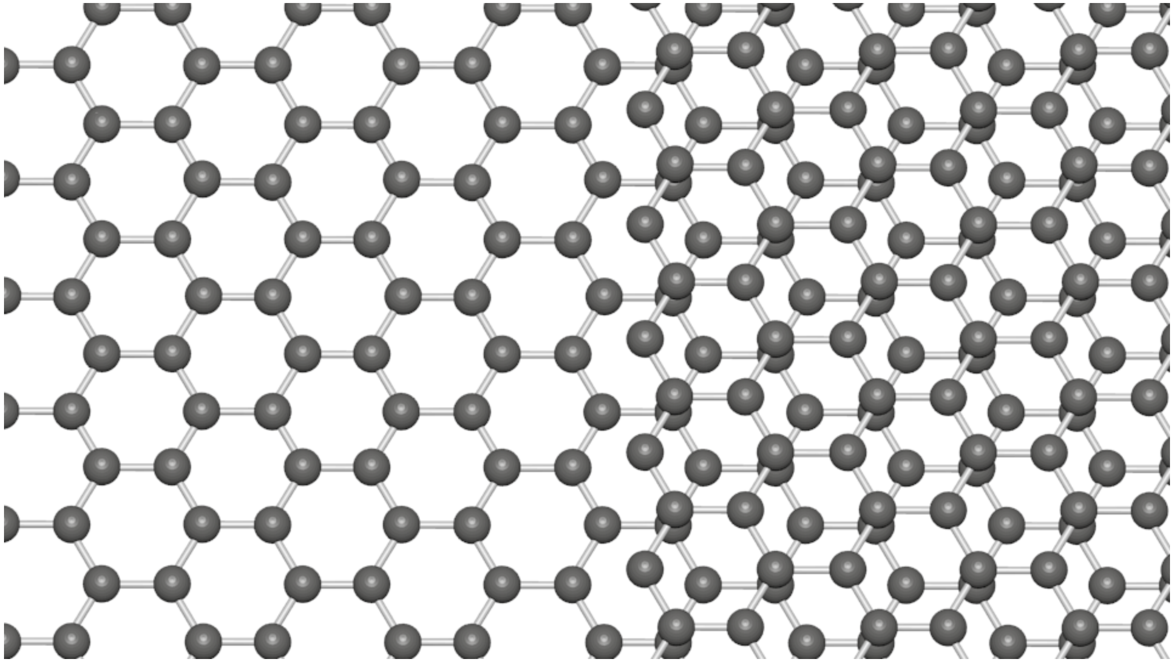
… Not yet realized

Kiselev and Kim, APL 78, 775 (2001).
Ohe et al, PRB 72, 041308 (2005).
Yamamoto et al, PRB72, 115321 (2005).

… Can we do this in better way in 2D materials ?

This talk: Electron transmission through atomic boundary

Graphene

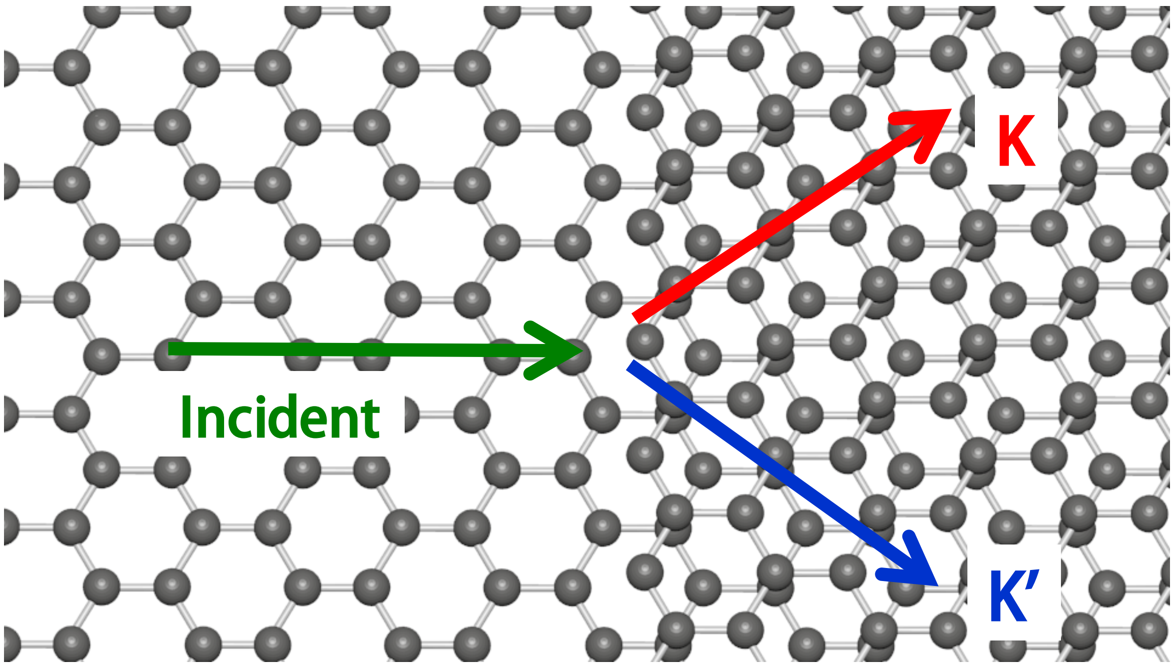


Monolayer

Bilayer (AB-stacked)

This talk: Electron transmission through atomic boundary

Graphene



Monolayer

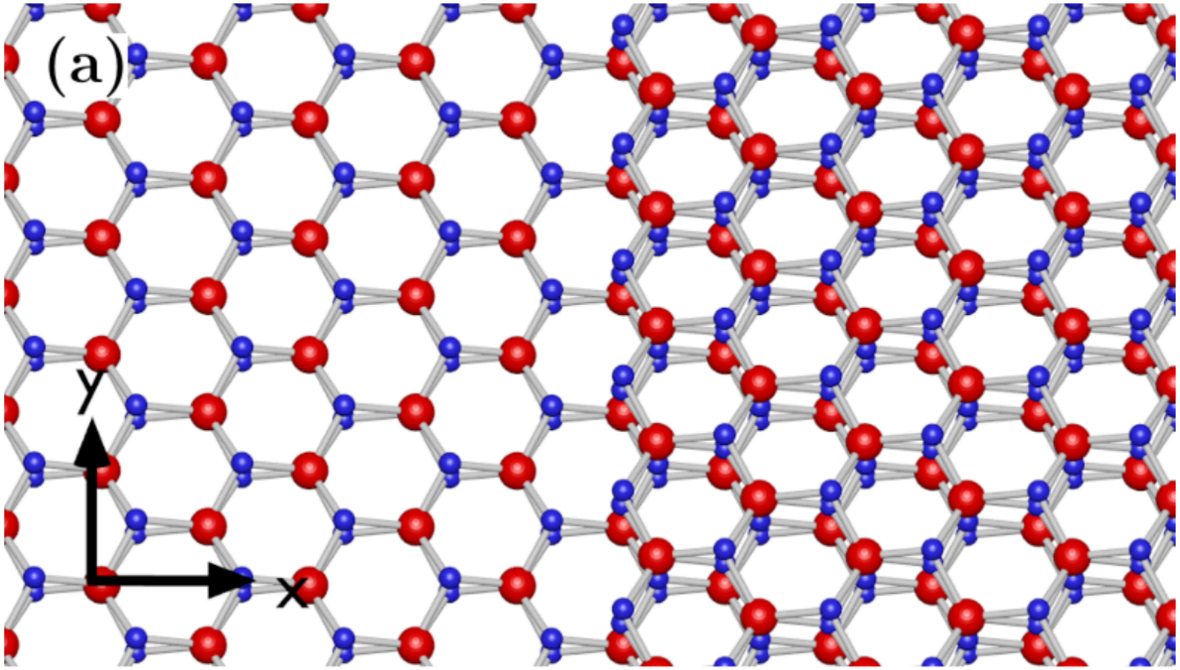
Bilayer (AB-stacked)

Graphene atomic boundary splits valley pseudo-spins (K,K')

This talk: Electron transmission through atomic boundary

Transition metal dichalcogenides (TMD)

MX_2 (M=Mo,W; X=S, Se,Te)

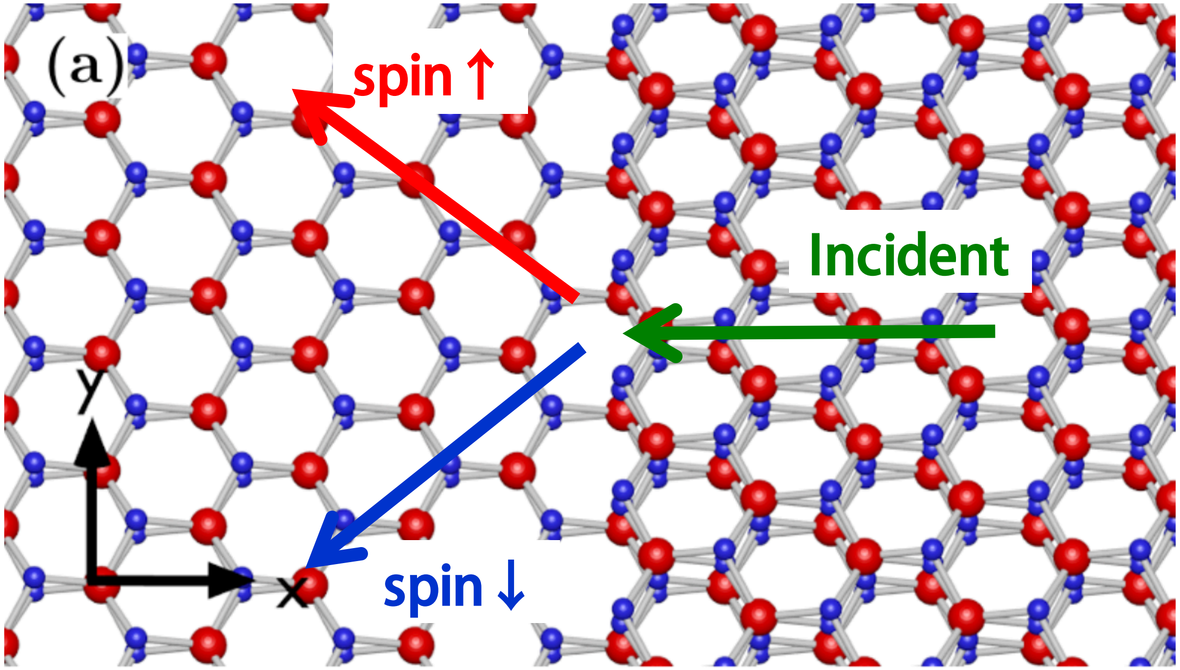


Monolayer Bilayer

This talk: Electron transmission through atomic boundary

Transition metal dichalcogenides (TMD)

MX_2 (M=Mo,W; X=S, Se,Te)



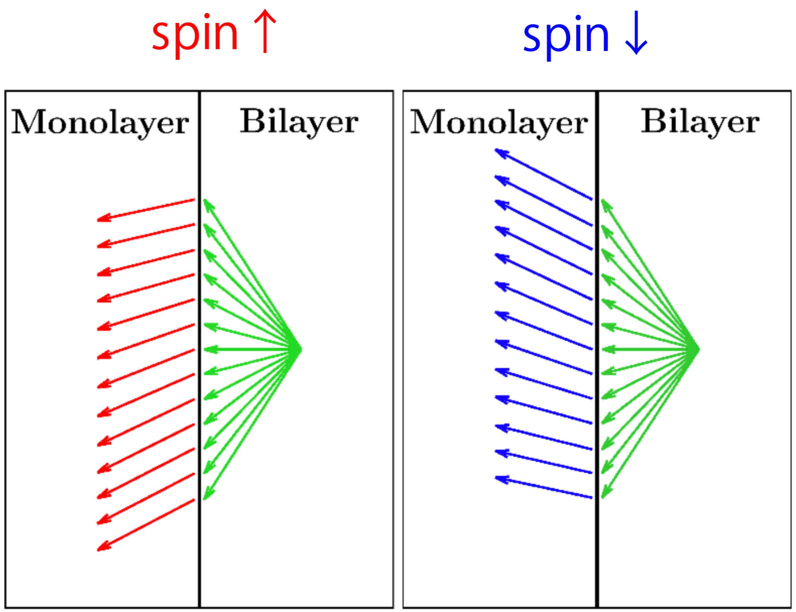
Monolayer

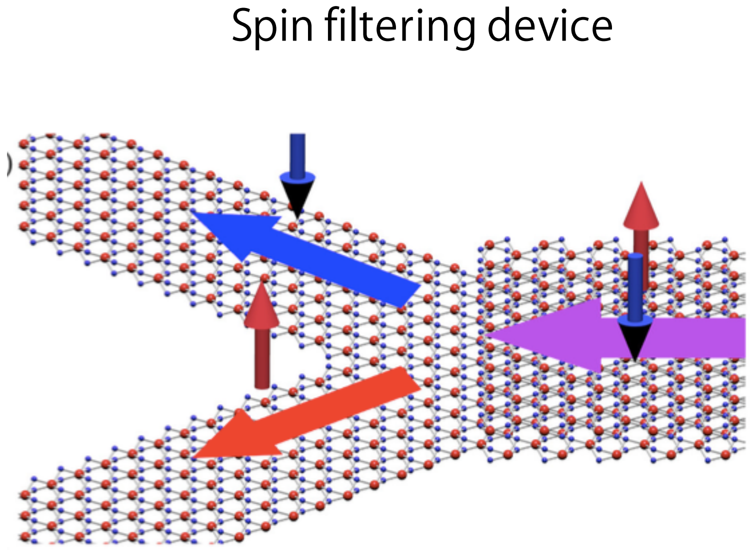
Bilayer

TMD atomic boundary splits real spins!

This talk: Electron transmission through atomic boundary

TMD monolayer-bilayer junction works as a spin splitter



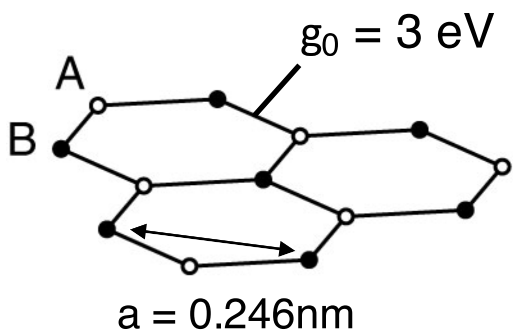


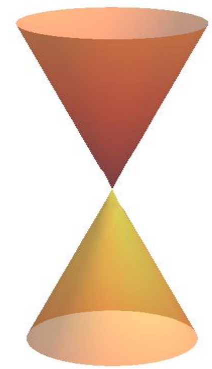
T. Habe and M. Koshino, Phys. Rev. B 91, 201407(R) (2015)

Graphene's band structure

Monolayer graphene

McClure, Phys. Rev. **104**, 666 (1956).





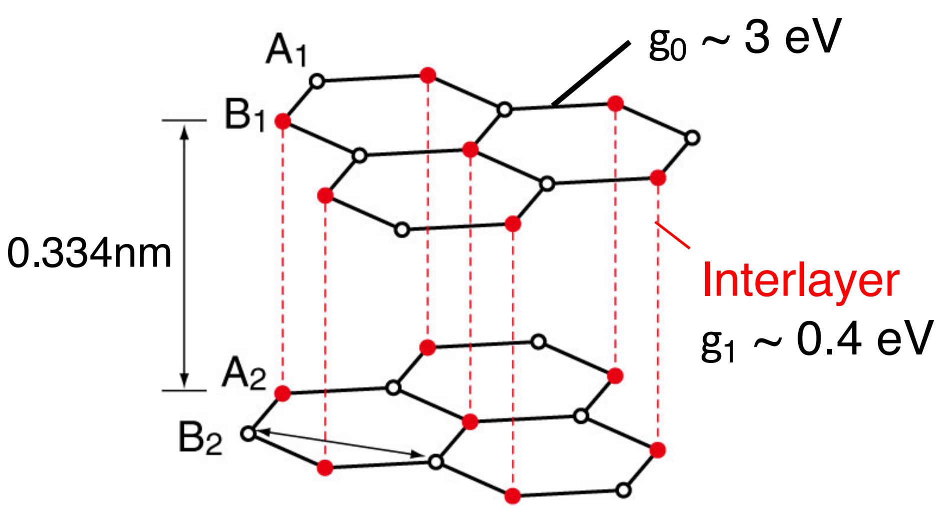
Linear

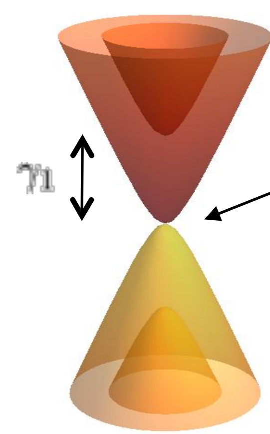
$$v = \frac{\sqrt{3}a}{2\hbar}\gamma_0 \approx 1 \times 10^6 \mathrm{m/s}$$

…. constant velocity

Bilayer graphene

McCann and Fal'ko, PRL **96**, 086805 (2006)





Massive

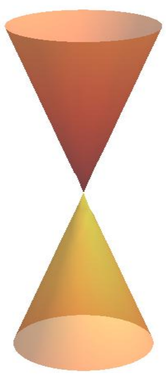
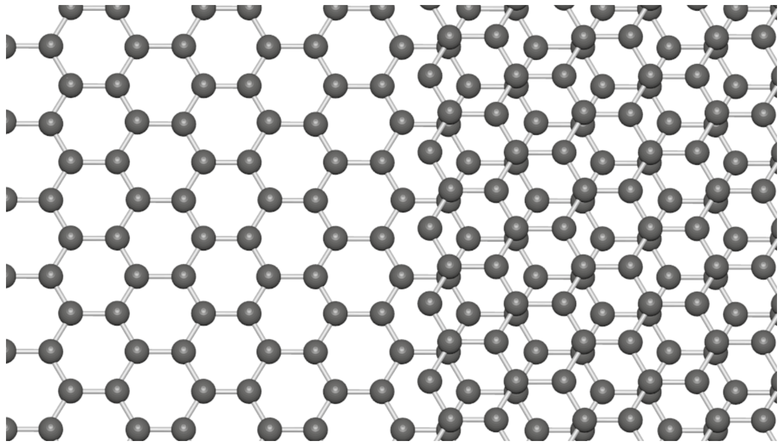
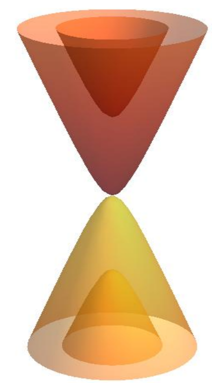
Effective mass:

$$m^* = \frac{\gamma_1}{2v^2} \sim 0.03 m_0$$

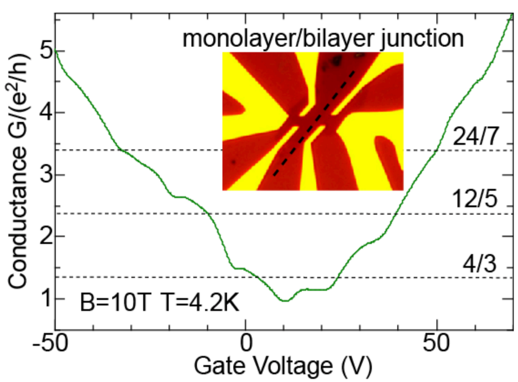
Graphene monolayer-bilayer junction

Theoretical studies

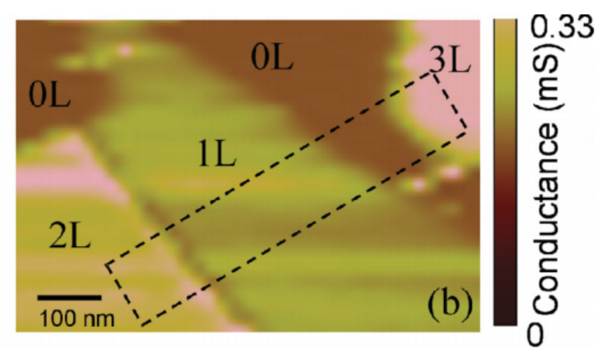
Nakanishi, Koshino, Ando, PRB **82**, 125428 (2010)
Koshino, Nakanishi, Ando PRB **82**, 205436 (2010)

Experiments



Tsukada et al, J. Phys.: Conf. Series 334, 012038 (2011)



Giannazzo et al, Phys. Rev. B 86, 235422 (2012)

Boundary condition in continuum model

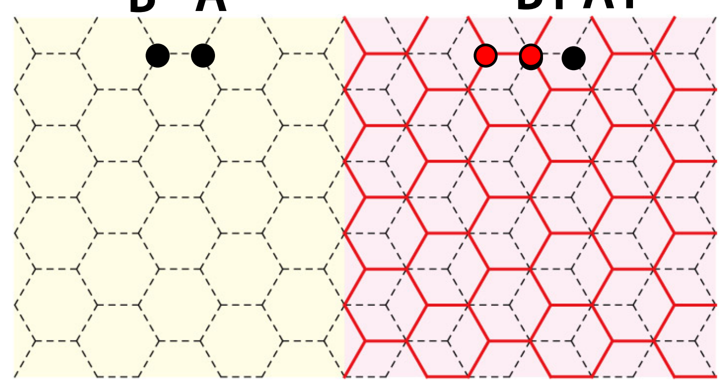
	Monolayer (K-valley)	Bilayer (K-valley)
Hamiltonian	$\mathcal{H}^K = \begin{pmatrix} 0 & vp_- \\ vp_+ & 0 \end{pmatrix}$ $p_\pm = p_x \pm ip_y$	$\mathcal{H}^K = \begin{pmatrix} 0 & vp_- & 0 & 0 \\ vp_+ & 0 & \gamma_1 & 0 \\ 0 & \gamma_1 & 0 & vp_- \\ 0 & 0 & vp_+ & 0 \end{pmatrix}.$
Wavefunction	$\mathbf{F}^K(\mathbf{r}) = \begin{pmatrix} F_A^K(\mathbf{r}) \\ F_B^K(\mathbf{r}) \end{pmatrix}$	$\mathbf{G}^K(\mathbf{r}) = \begin{pmatrix} G_{A1}^K(\mathbf{r}) \\ G_{B1}^K(\mathbf{r}) \\ G_{A2}^K(\mathbf{r}) \\ G_{B2}^K(\mathbf{r}) \end{pmatrix}$

Boundary condition (Zigzag-1)

$$F_A^K(0,y) = G_{A1}^K(0,y)$$
$$F_B^K(0,y) = G_{B1}^K(0,y)$$

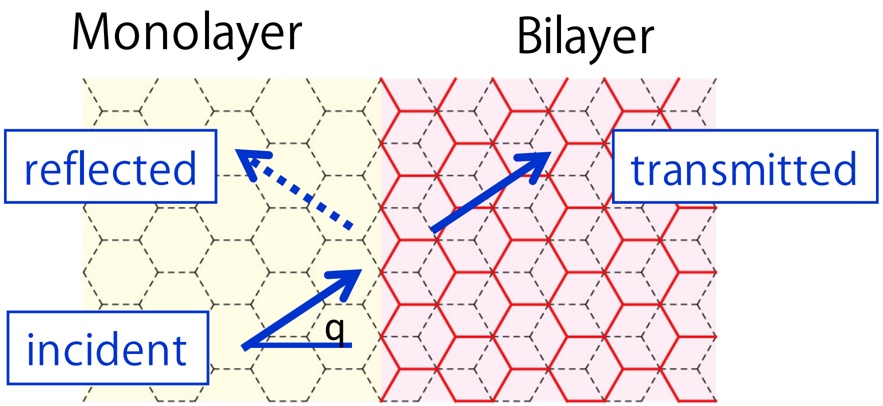
} 1st layer

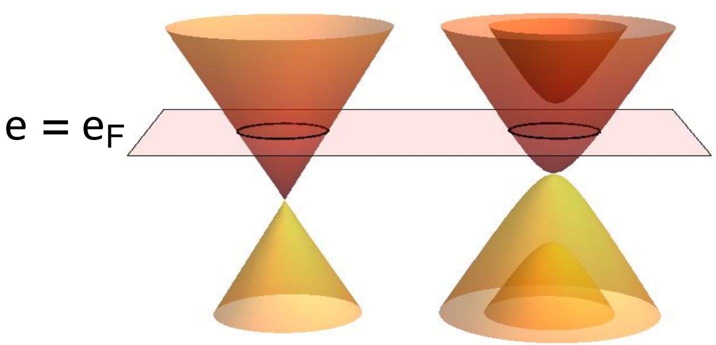
$$0 = G_{B2}^K(0,y)$$ — 2nd layer

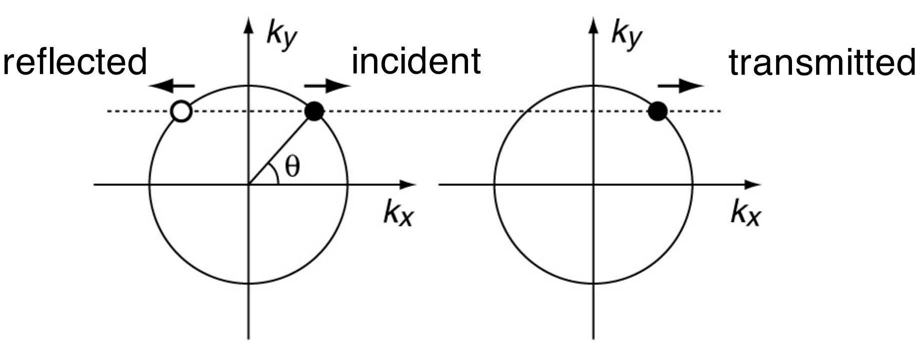


Transmission through M-B junction

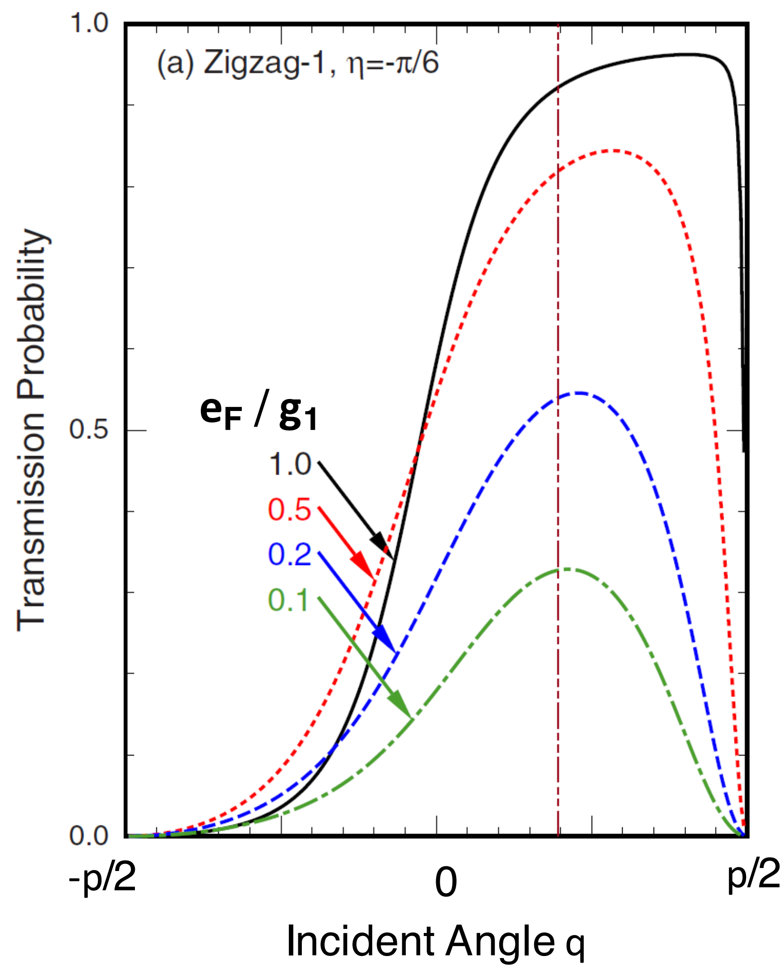
T. Nakanishi, MK, T. Ando
PRB **82**, 125428 (2010)







Transmission Probability (K-valley)



Transmission through M-B junction

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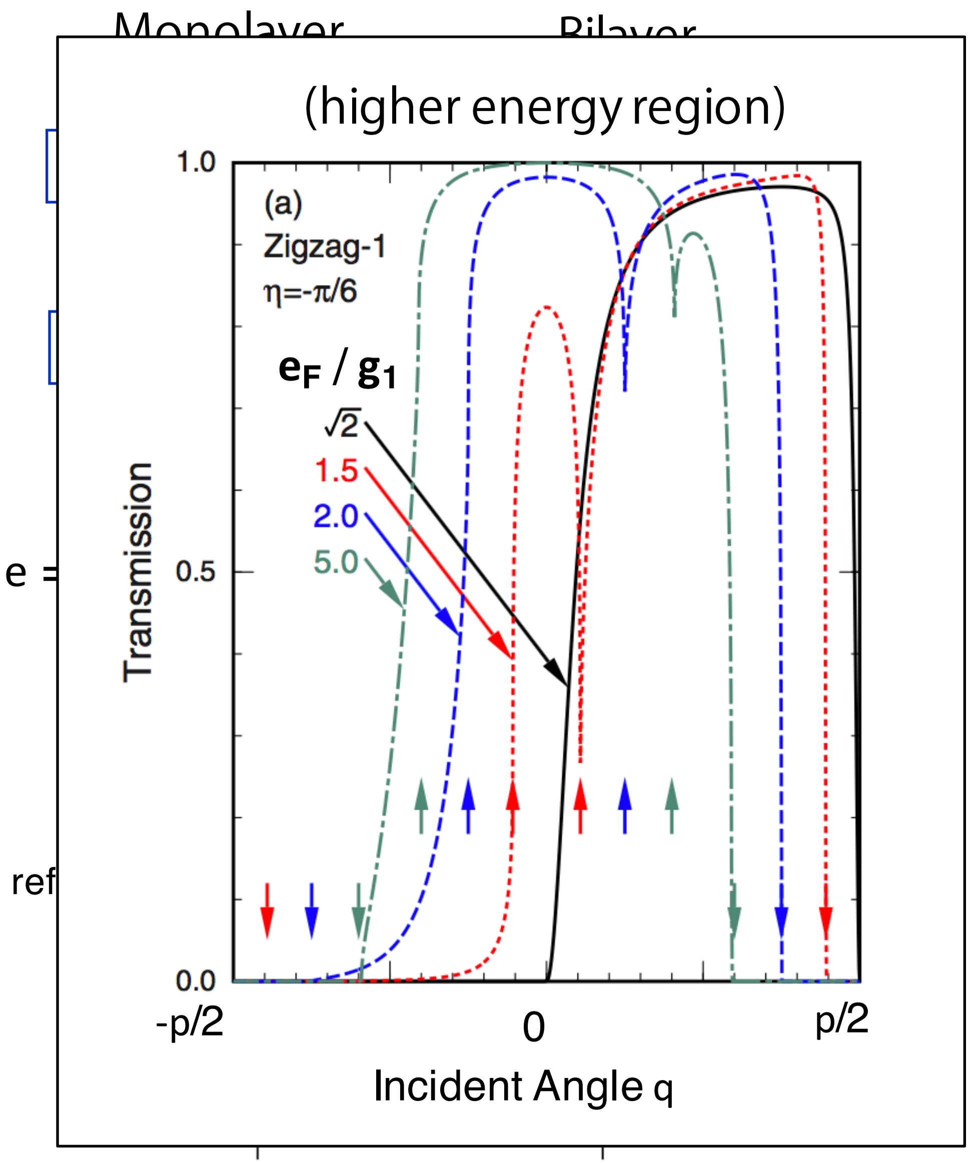
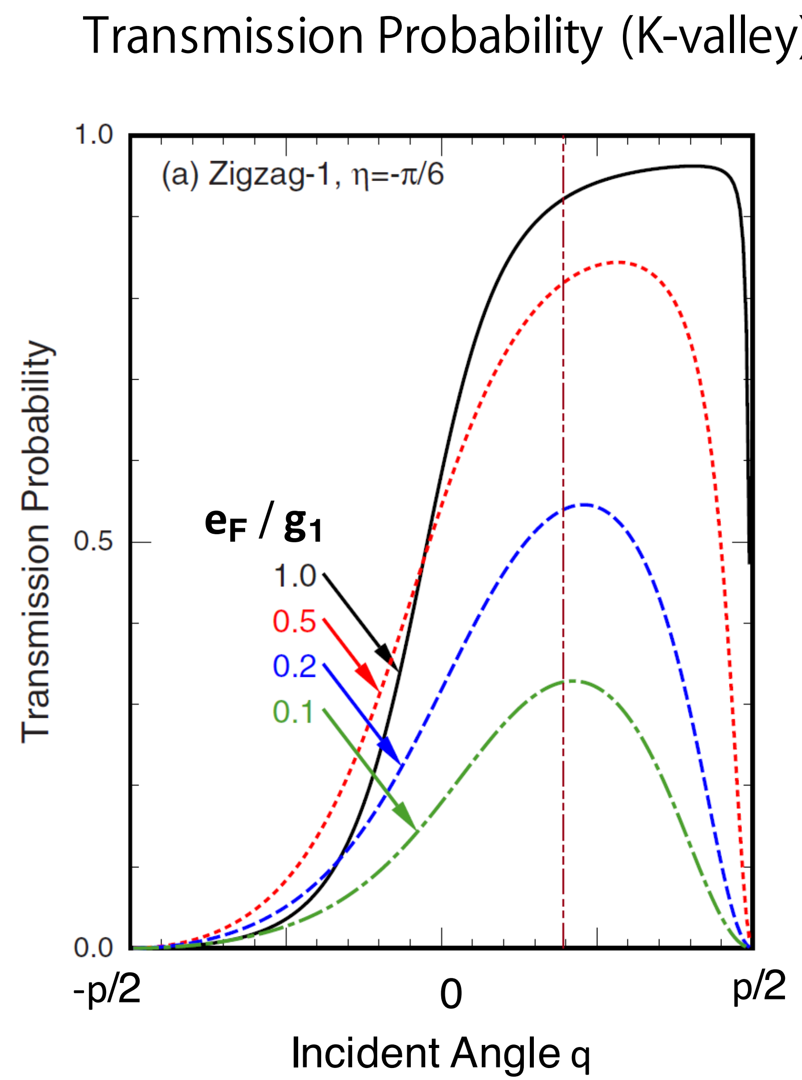
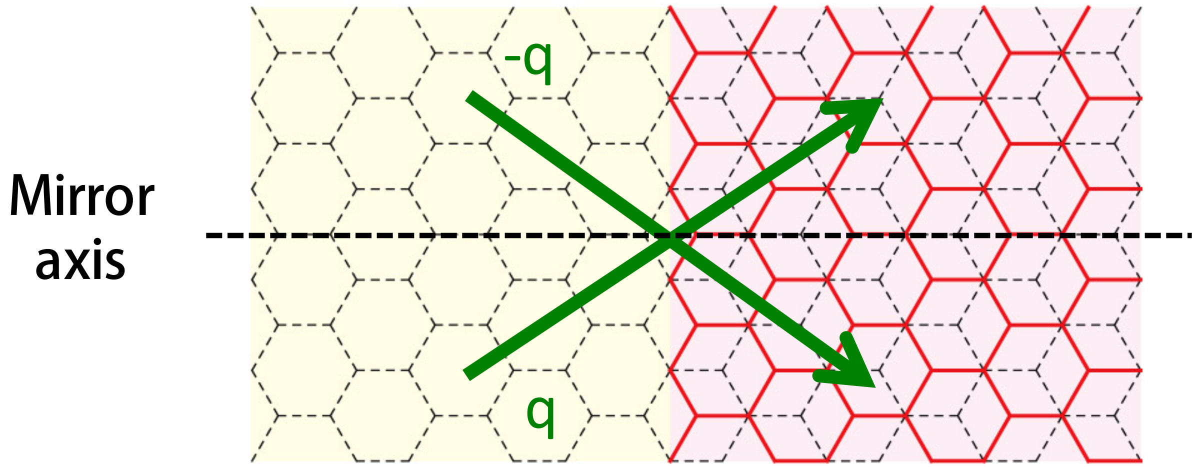




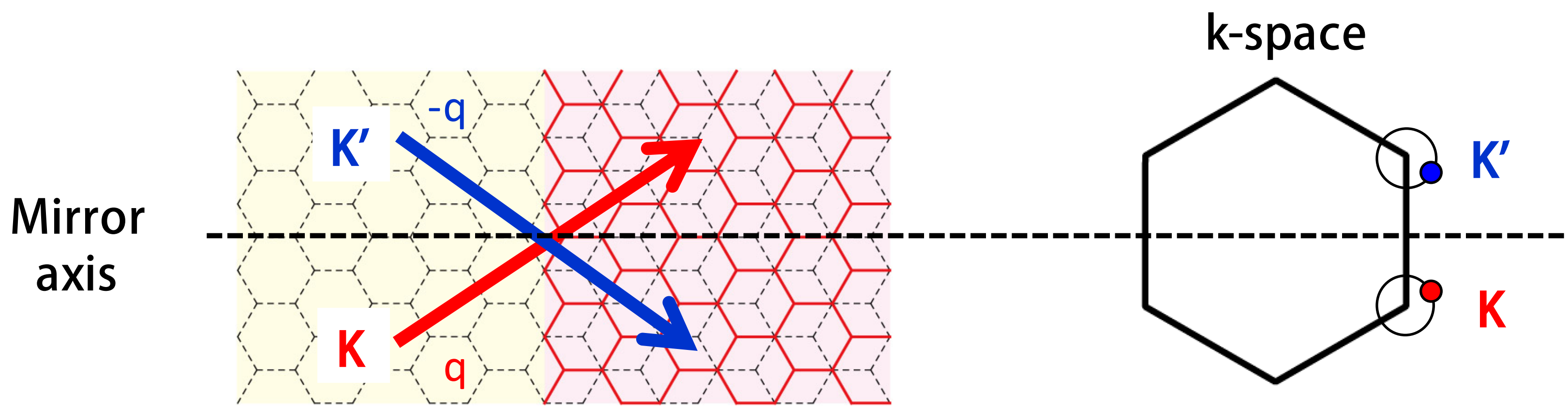
Why angle-asymmetric?



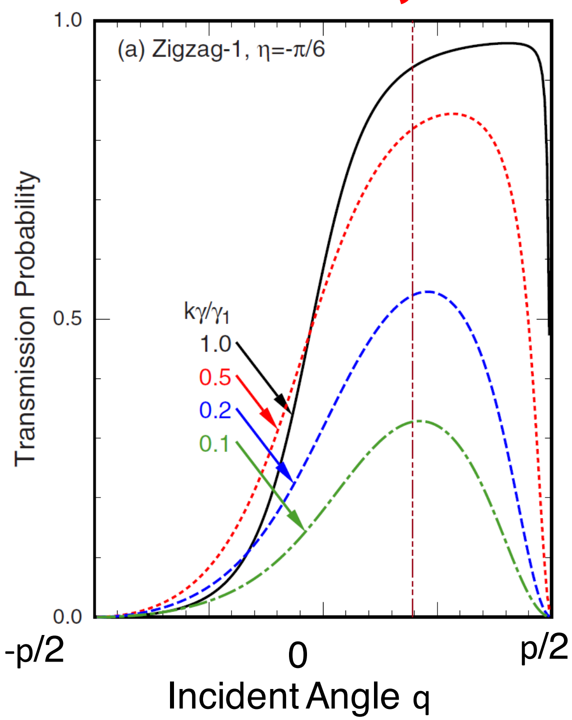
Mirror symmetry

··· Transmission should be symmetric with respect to $\mathbf{q} = 0$?

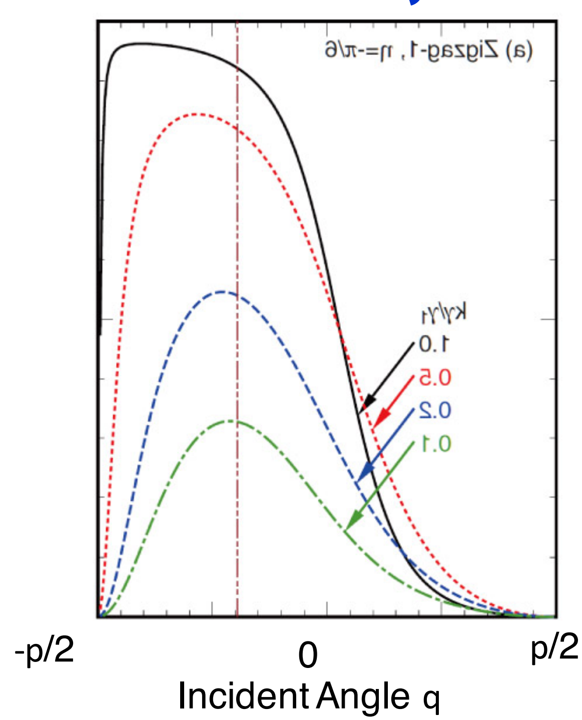
Why angle-asymmetric?



K-valley

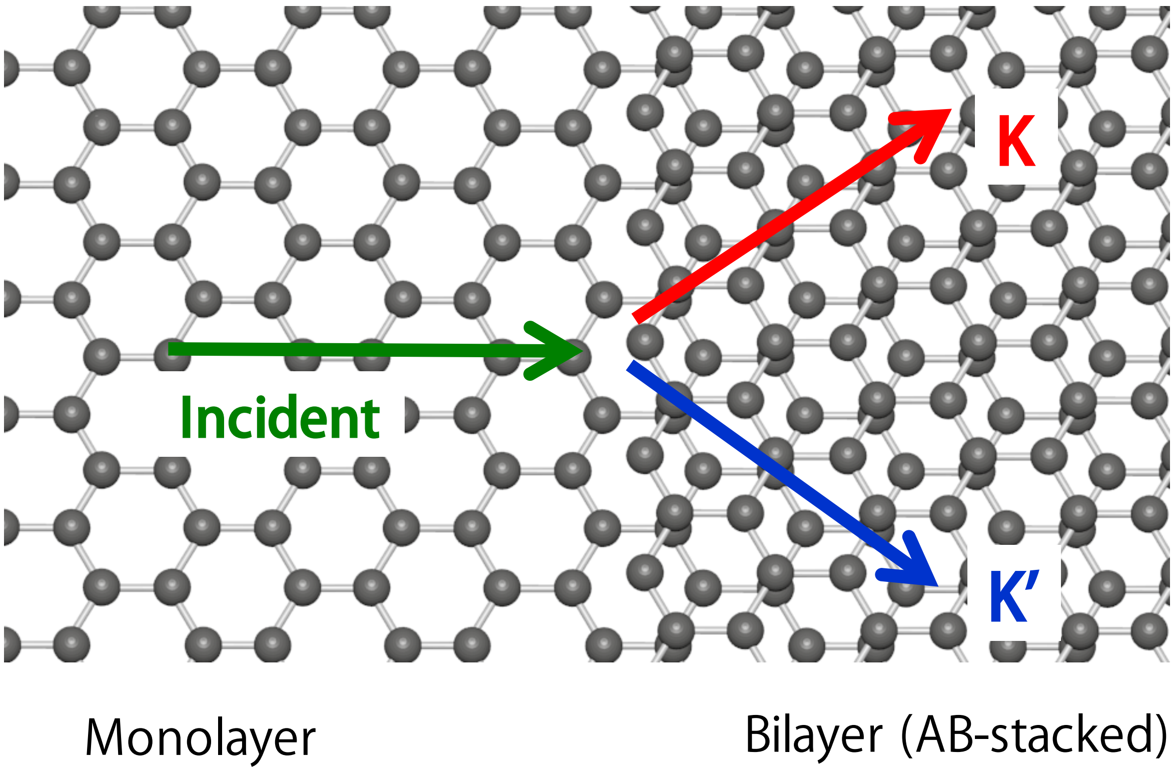


K'-valley



Asymmetric transmission in K and K'

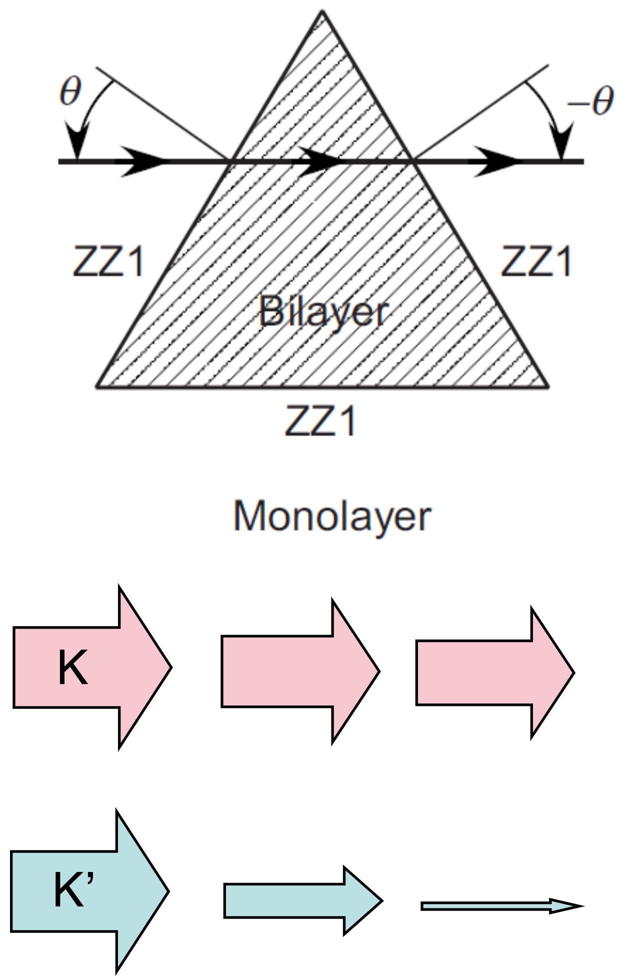
Graphene



Graphene atomic boundary splits valley pseudo-spins (K,K')

Valley-polarizing mechanism

T. Nakanishi, MK, T. Ando
PRB **82**, 125428 (2010)

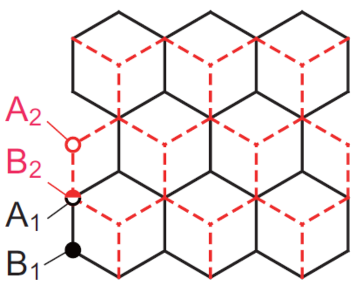


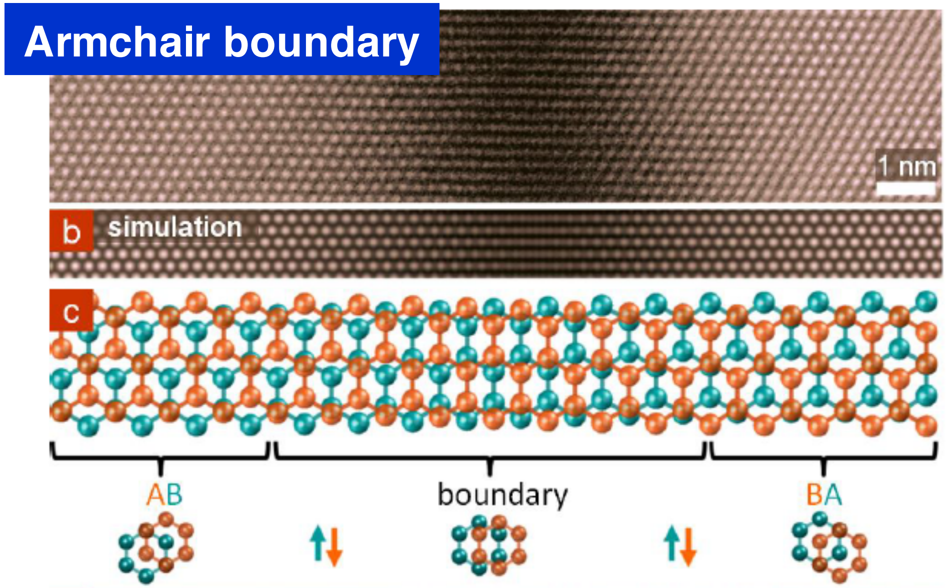
Valley polarization

AB-BA domain in bilayer graphene

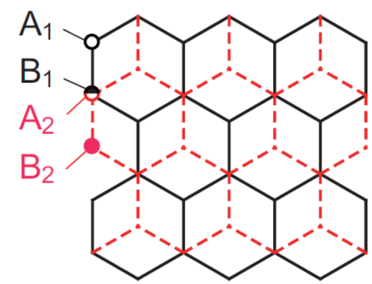
J. S. Alden et al,
PNAS
110, 11256 (2013)

AB

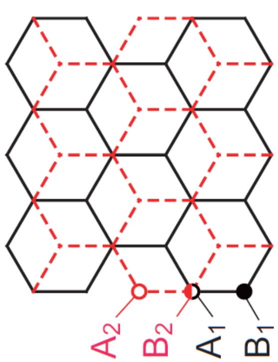


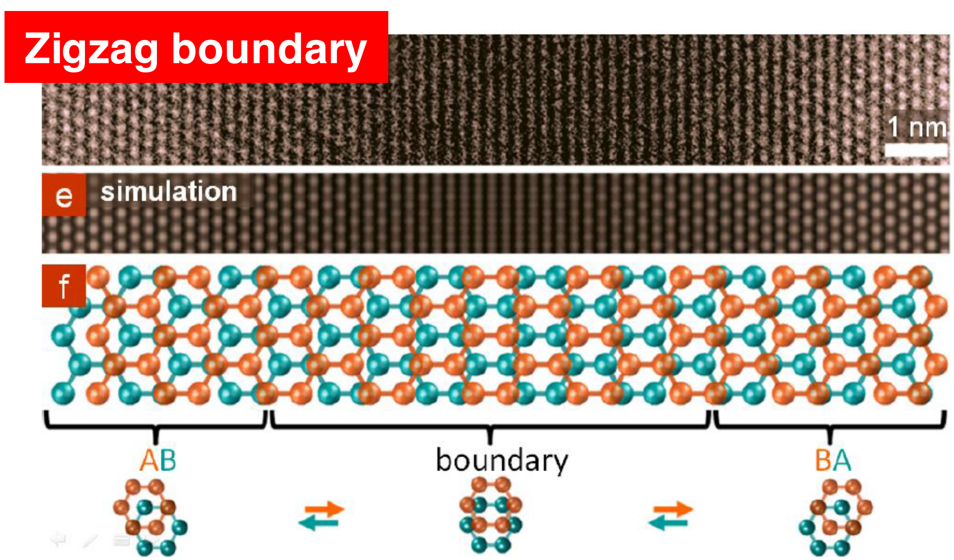


BA

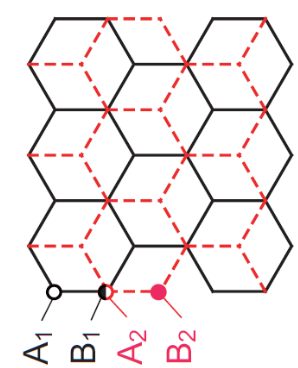


AB





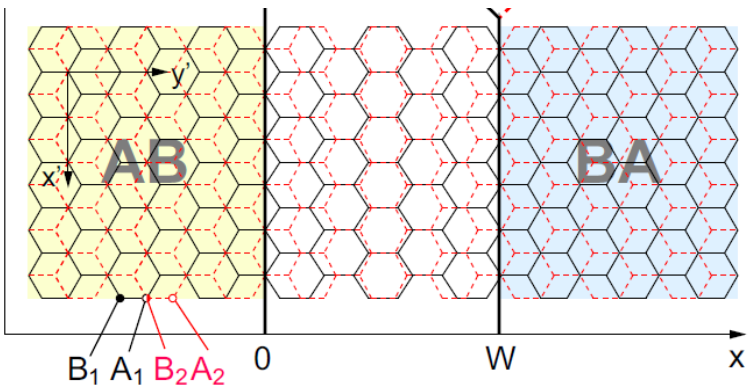
BA

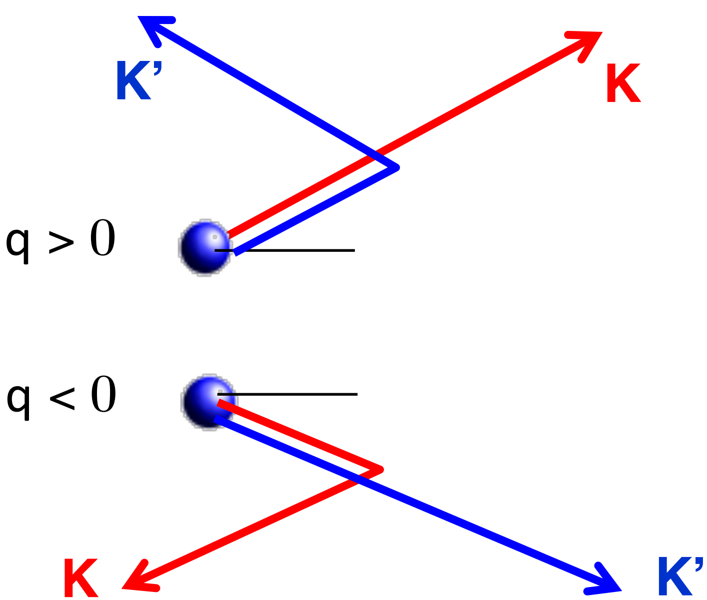


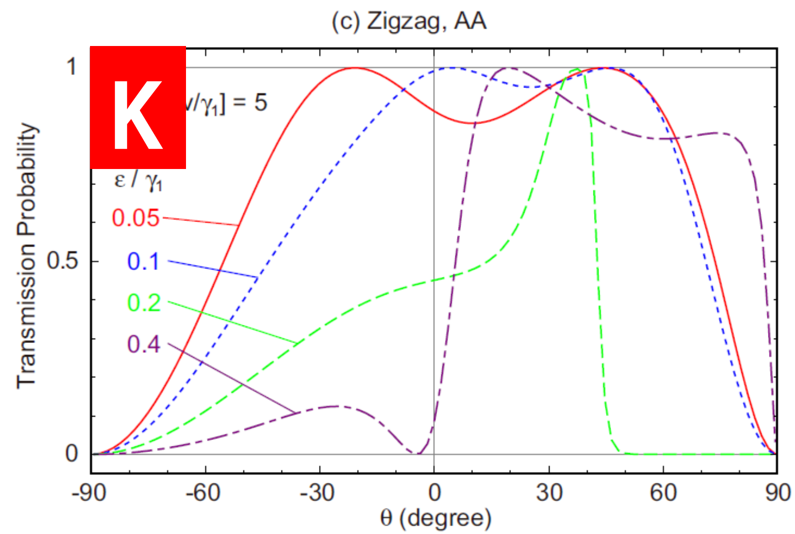
Valley polarization

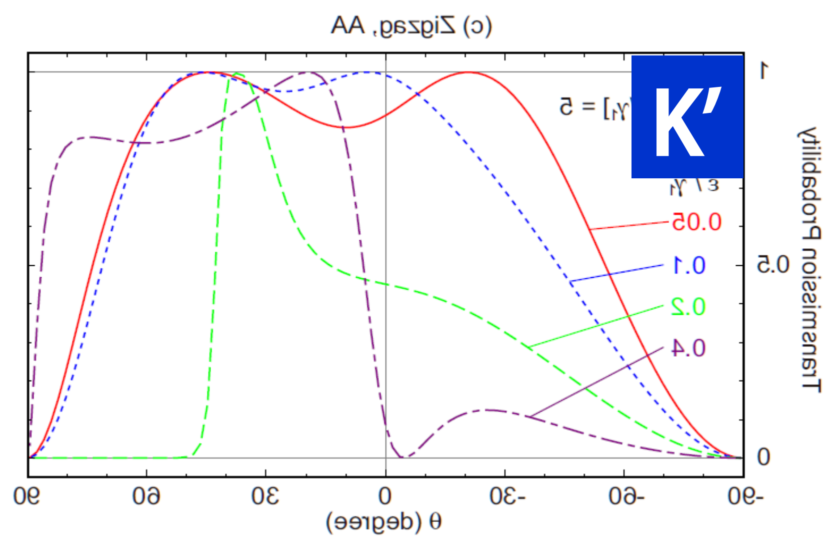
M. Koshino,
Phys. Rev. B 88, 115409 (2013)

Reflection symmetry: K and K’ have opposite angle dependence

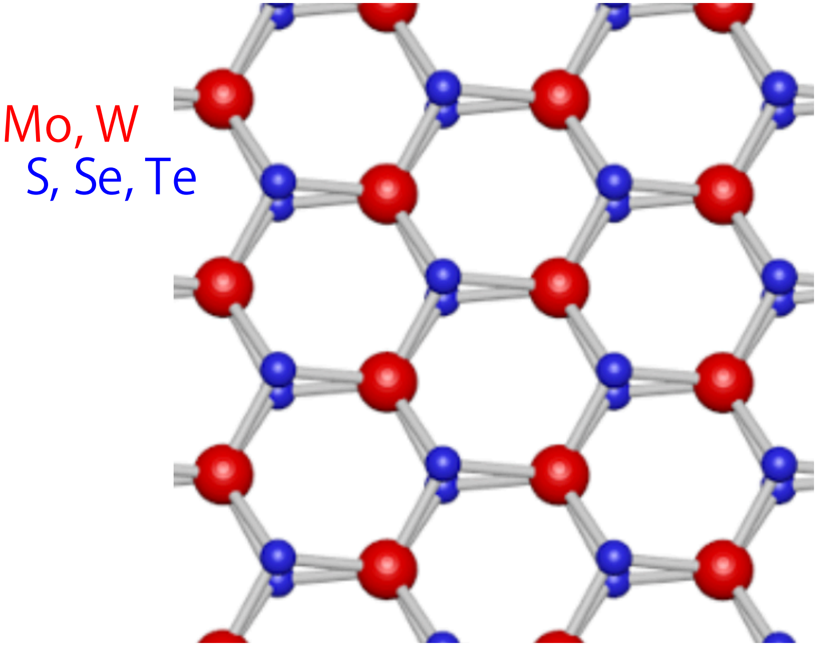




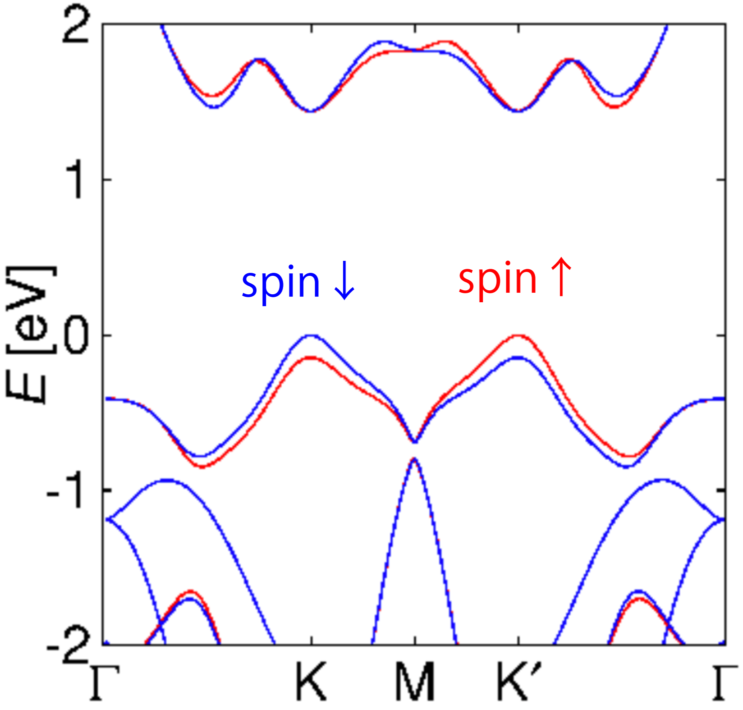




TMD (Transition metal dichalcogenides)



Band structure ($MoSe_2$)



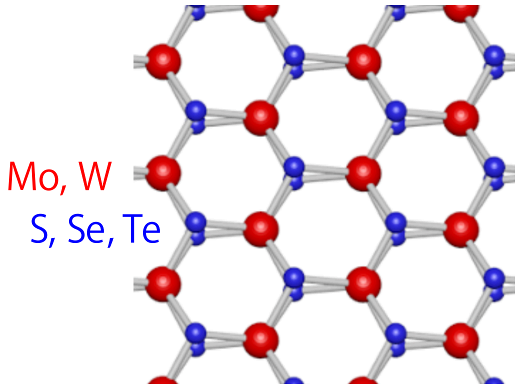
Inversion symmetry breaking
+
Spin-orbit coupling

Spin split
(opposite in K and K′)

K. F. Mak, et al, Nat. Nano. 7, 494 (2012), D. Xiao, et al, PRL 108, 196802 (2012).

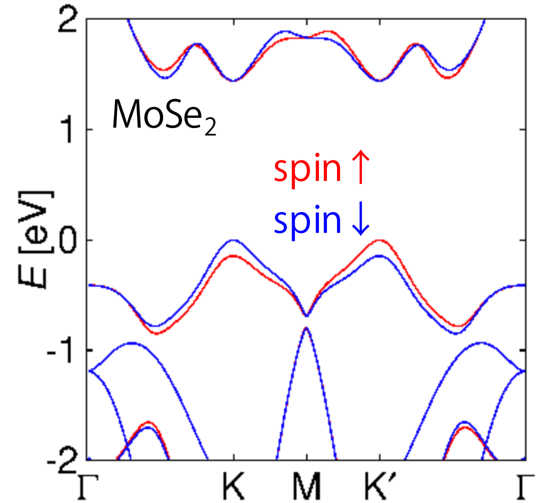
TMD (Transition metal dichalcogenides)

Monolayer

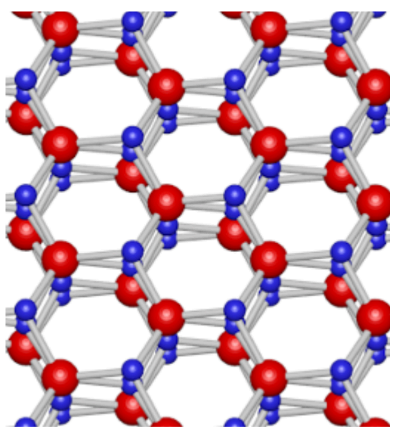


Inversion symmetry breaking
+
Spin-orbit coupling

Spin split

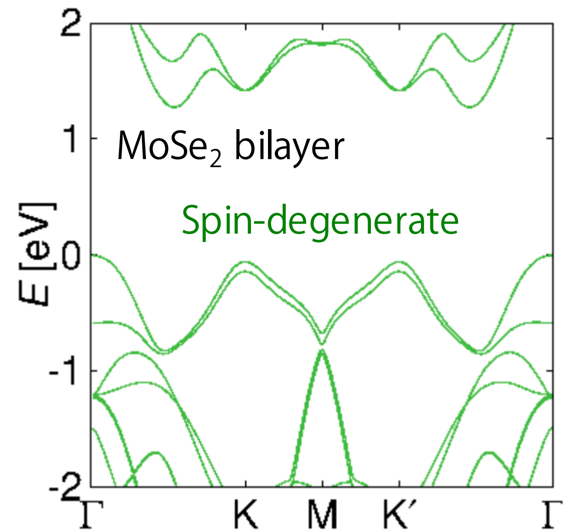


Bilayer (2H phase)



Inversion symmetry recovers

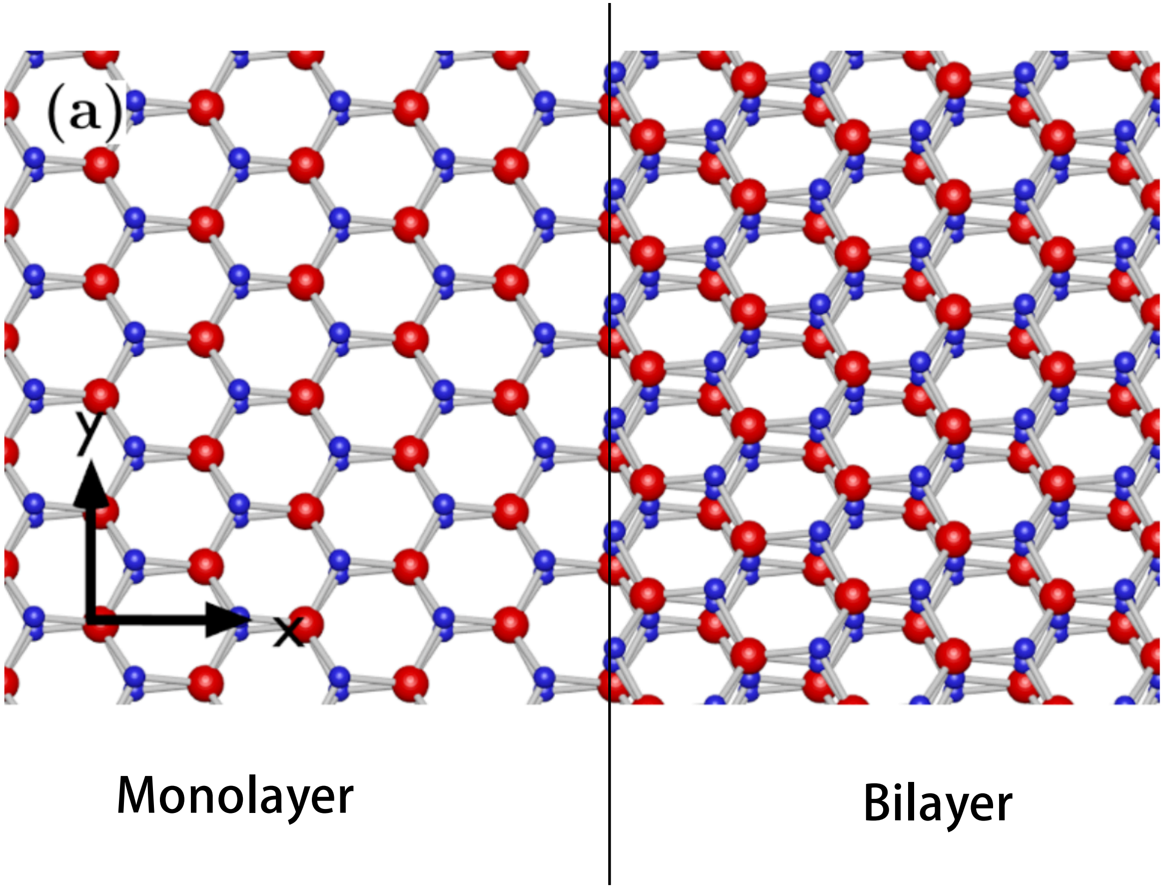
Spin degenerate



K. F. Mak, et al, Nat. Nano. 7, 494 (2012), D. Xiao, et al, PRL 108, 196802 (2012).

TMD atomic junciton

T. Habe and M. Koshino,
Phys. Rev. B 91, 201407(R) (2015)



Monolayer

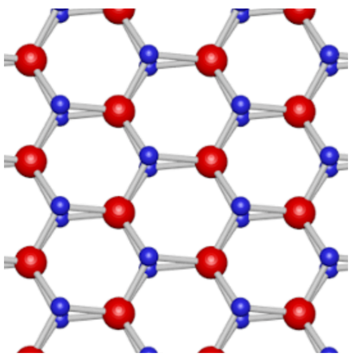
Bilayer

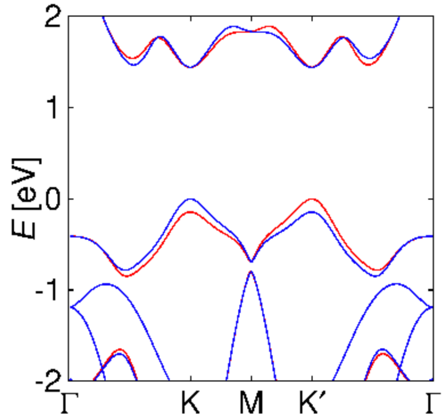
Zigzag edge

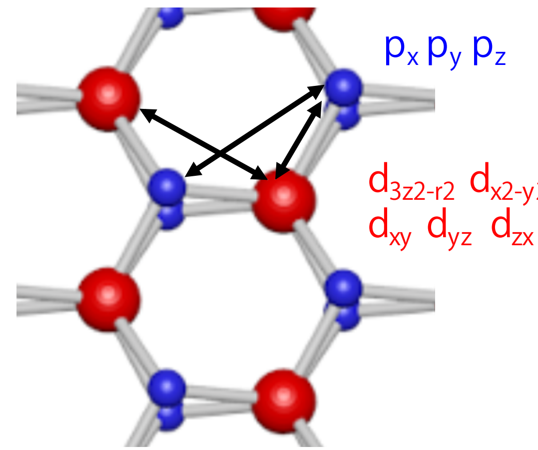
Theoretical Method

i) DFT band calculation
(Quantum Espresso)

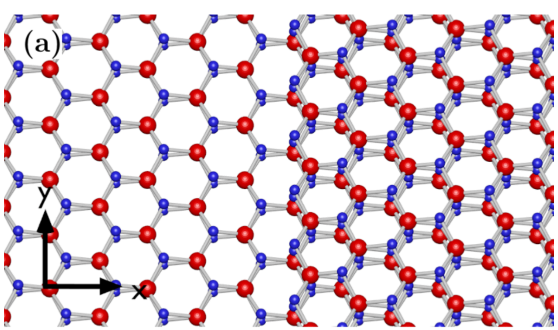
ii) Create tight-binding model
(Wannier 90)

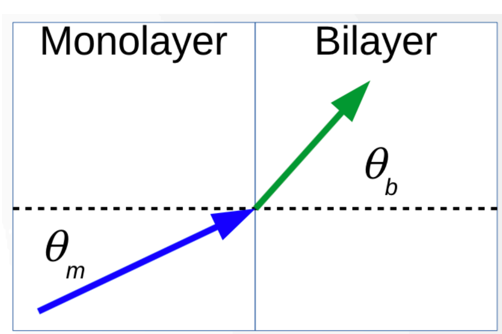


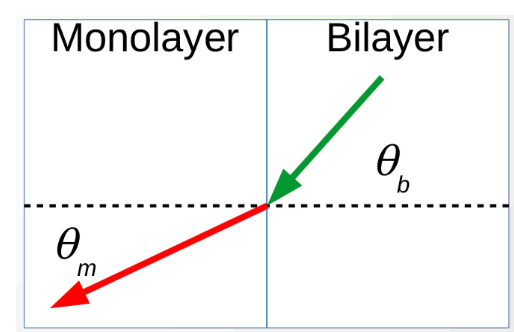




iii) Calculate the transmission probability



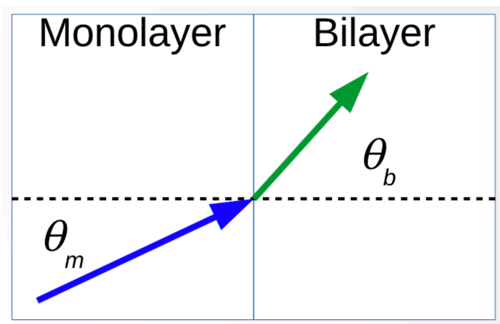




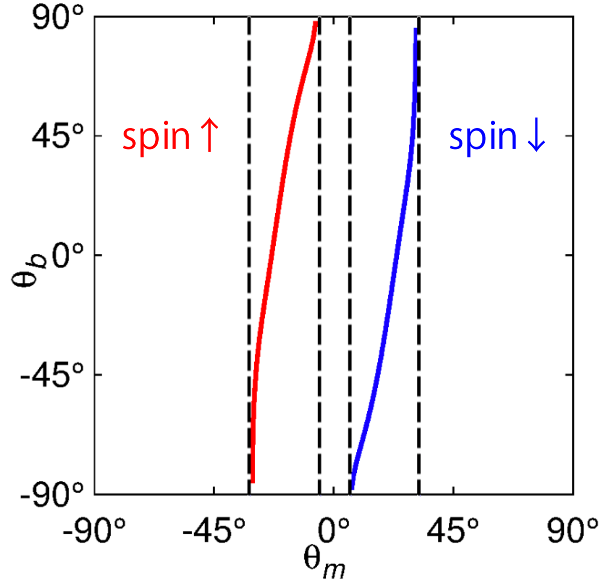
Electron transmission: $MoTe_2$

[hole-doped;
n=-7.02x10^{13} cm^{-2}]

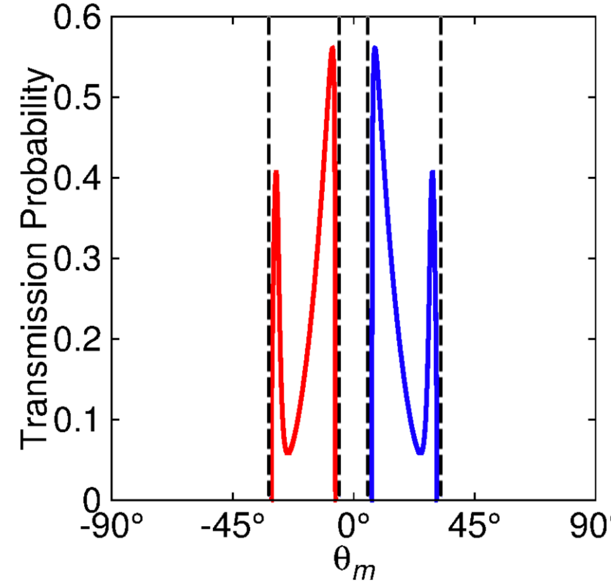
From monolayer side



Transmission angle

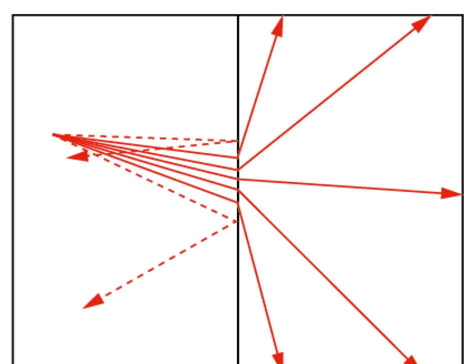


Transmission probability

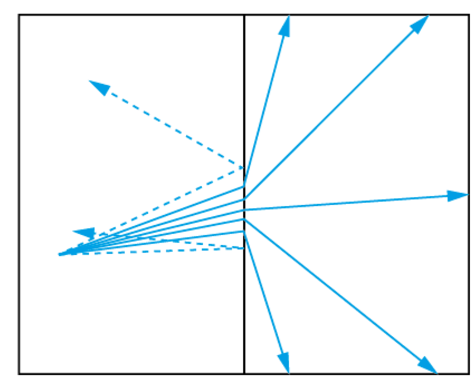


Transmission is
highly angle-selective

spin ↑



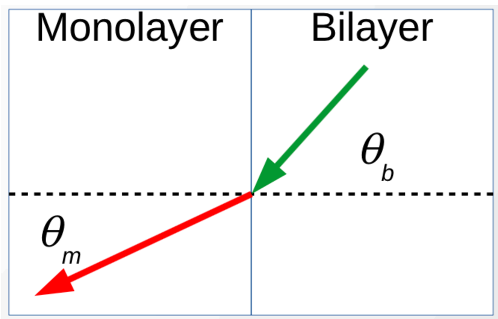
spin ↓

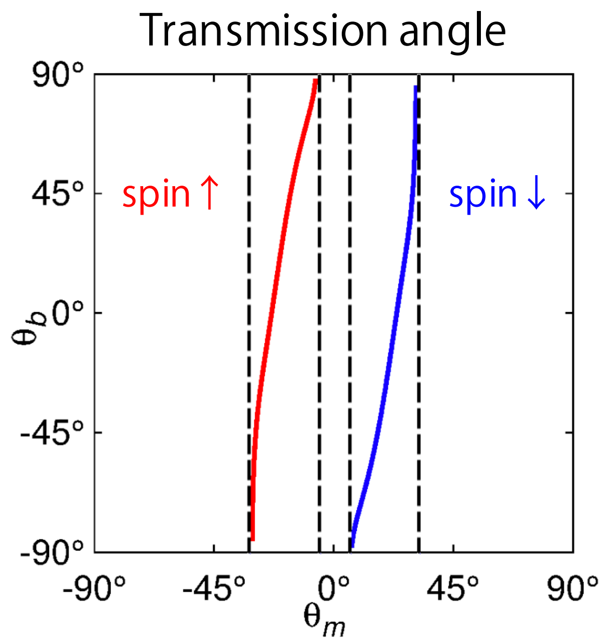


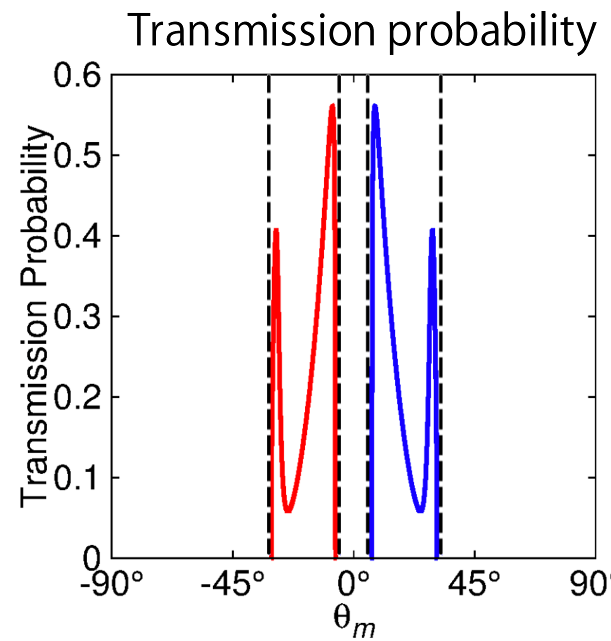
Electron transmission: $MoTe_2$

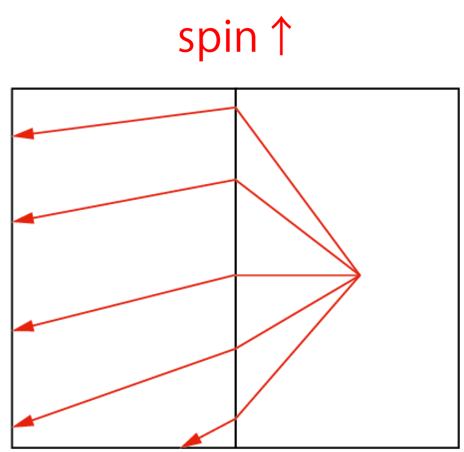
[hole-doped;
n=-7.02x10^{13} cm^{-2}]

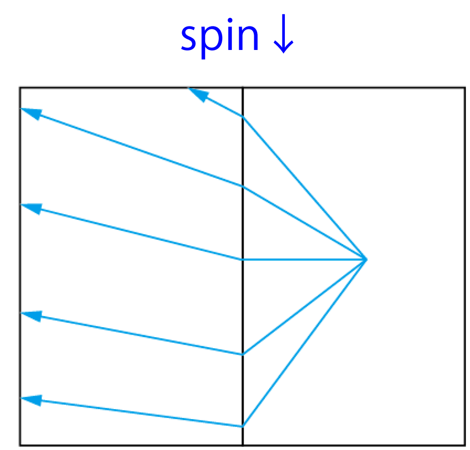
From bilayer side







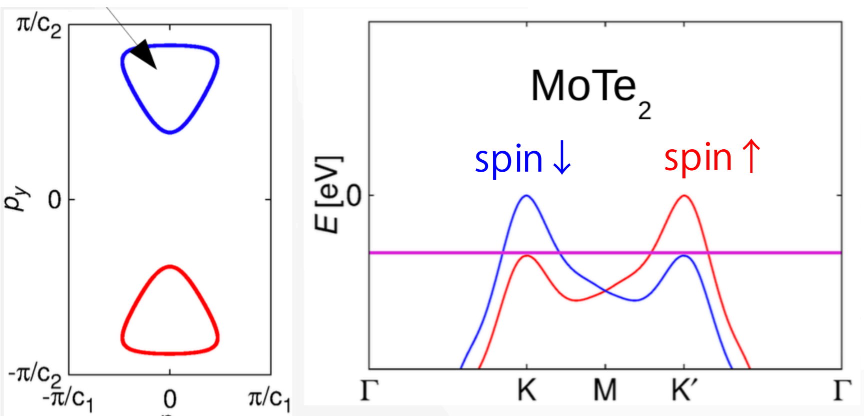


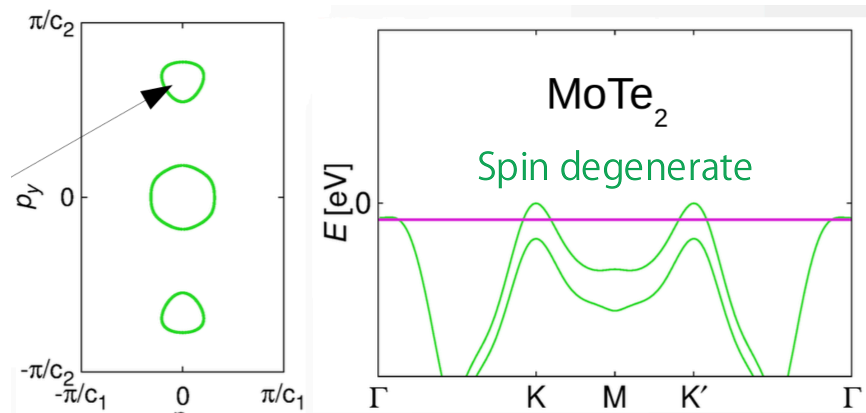


Collimated to different directions
depending on spin!

Mechanism of spin-dependent transmission

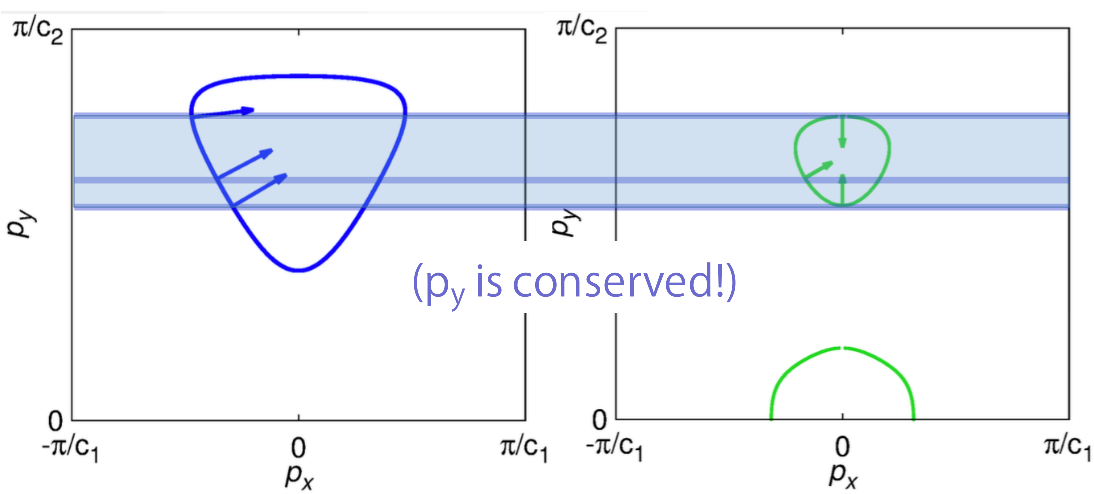
Monolayer ← (equal carrier density) → **Bilayer**

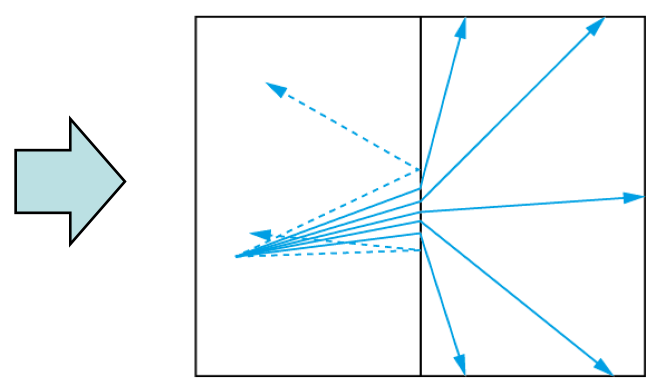




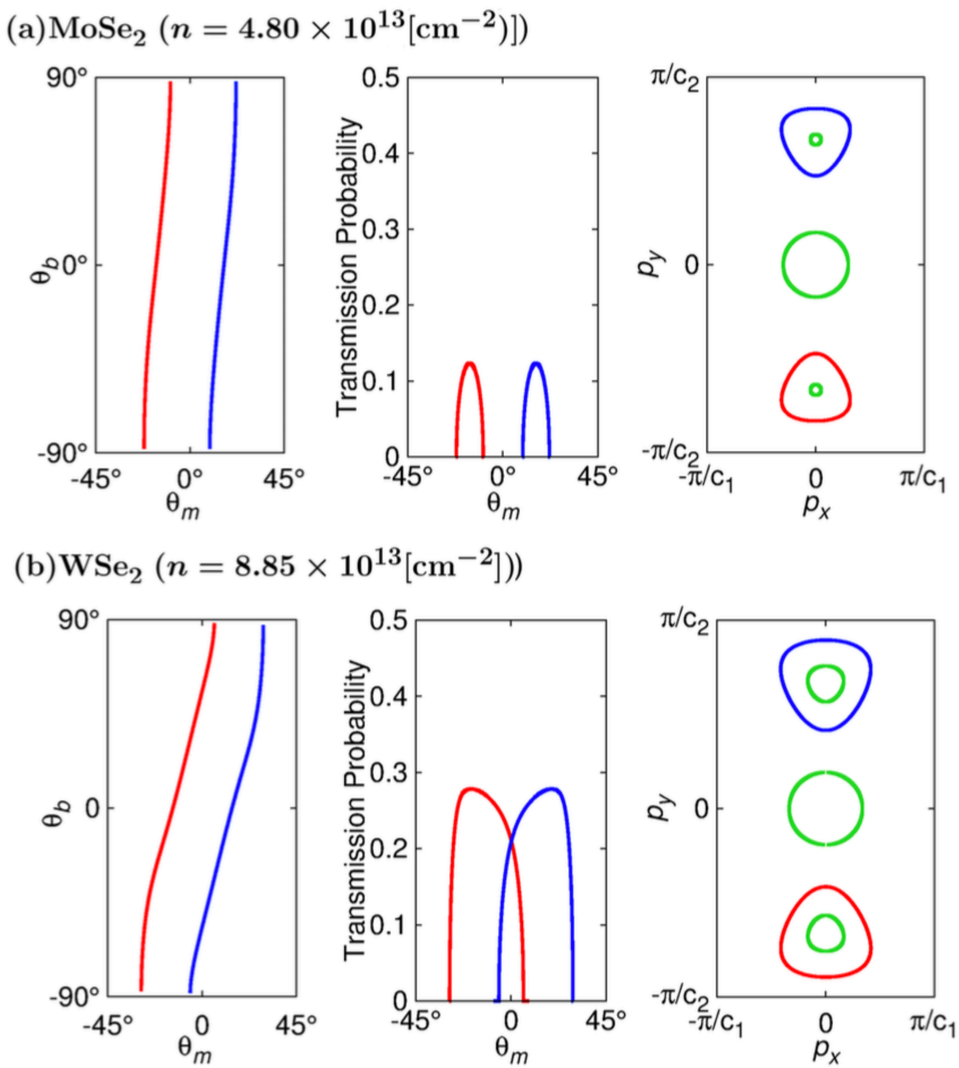
··· Larger Fermi circle in monolayer than in bilayer

Wave number matching





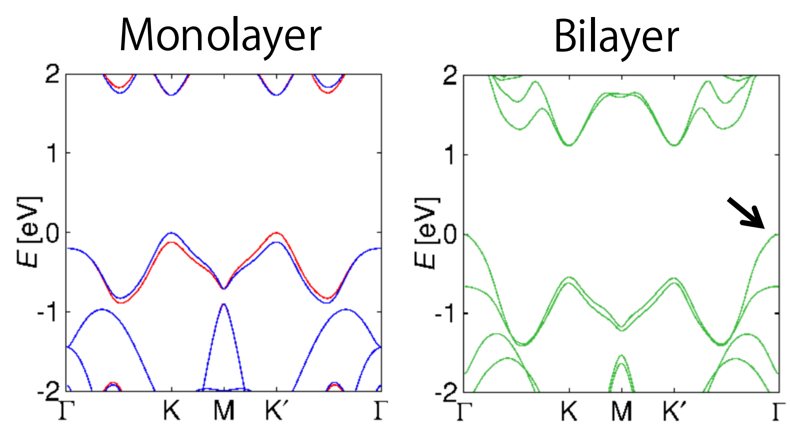
Other TMDs



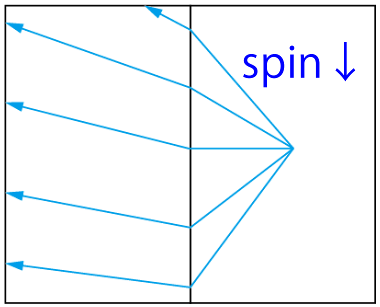
… Similar effects

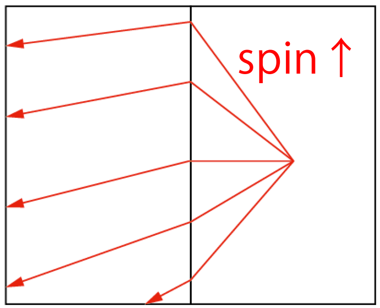
… MoS$_2$?

NO transmission at the boundary due to too high G point

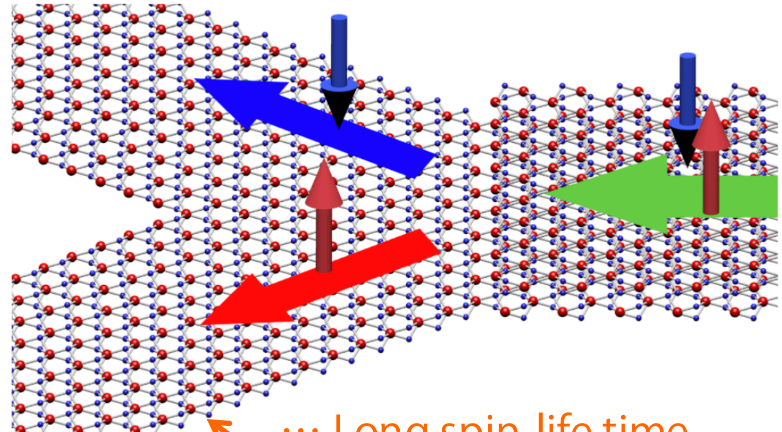


Spin splitter



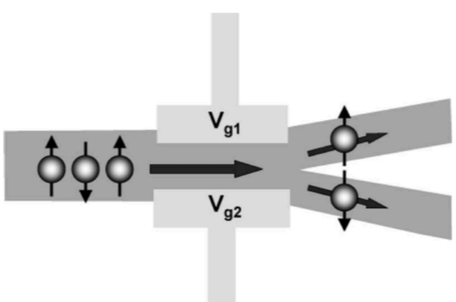


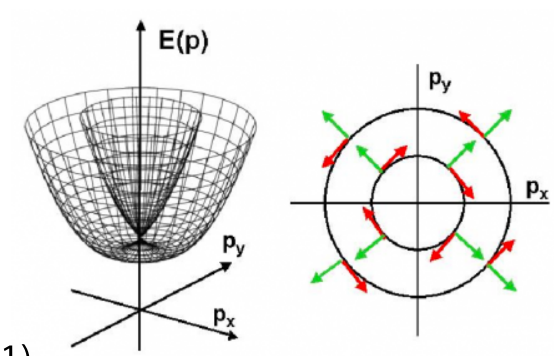
Monolayer Bilayer



… Long spin-life time
in monolayer region

Cf. spin splitters proposed in conventional 2DEG (Rashba spin-orbit interaction)





… Spin is not a conserved quantity
under impurity scattering

Kiselev and Kim, APL 78, 775 (2001).
Ohe et al, PRB 72, 041308 (2005).
Yamamoto et al, PRB72, 115321 (2005).

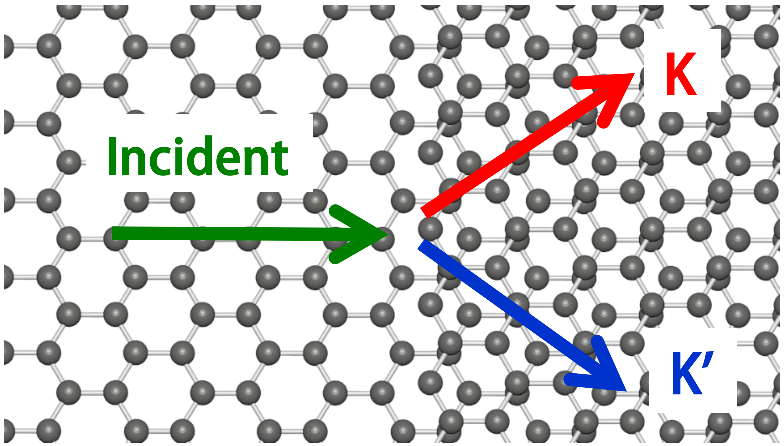
Summary

--- Atomic boundary in 2D material causes flavor-dependent electron transmission

--- Graphene mono-bi junction splits valley pseudospins

--- **TMD** ($MoSe_2$, $MoTe_2$, WSe_2, WTe_2) mono-bi junction splits real spins

--- Possible application to spin-filtering devices



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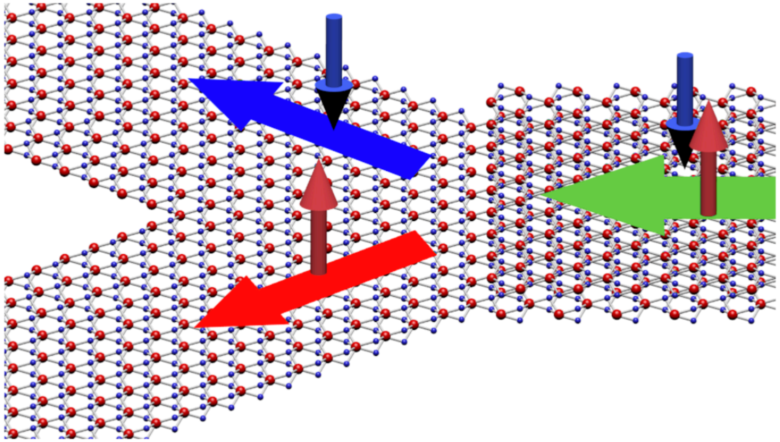
PRB **82**, 125428 (2010)



T. Habe and M. Koshino,
Phys. Rev. B 91, 201407(R) (2015)

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Dependence on edge configuration

T. Nakanishi, MK, T. Ando
PRB **82**, 125428 (2010)