2D Materials with Strong Spin-orbit Coupling: Topological and Electronic Transport Properties

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Topological insulators

Timeline

- **1975-1981** (Nobel prize 1985) Quantum Hall effect
- **2005** Quantum spin Hall (QSH) effect, topological order
- **2006** First realization in HgTe quantum wells

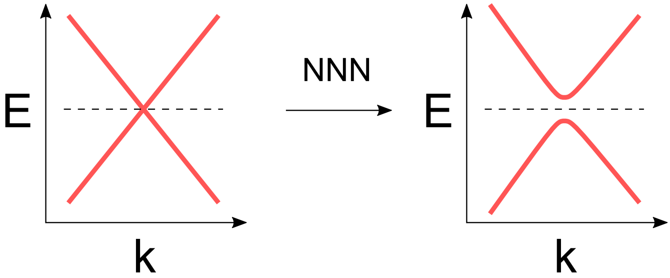
Materials?

The QSH effect in 2D

Kane-Mele model

$$H = \sum_{\text{spin}} \left[\sum_{\text{NN}} t_{\text{NN}} \cdot c^\dagger c + \sum_{\text{NNN}} i\nu t_{\text{NNN}} \cdot c^\dagger c \right]$$

Tight-binding model of graphene



Spin-orbit coupling

Spin-orbit coupling

Increases with atomic number Z:

$$\Delta_{SO} \sim \frac{Z^2}{n^3 l(l+1)}$$

Valence shells in carbon:

$$\Delta_{SO} < meV$$

Too small for spectroscopic and transport measurements

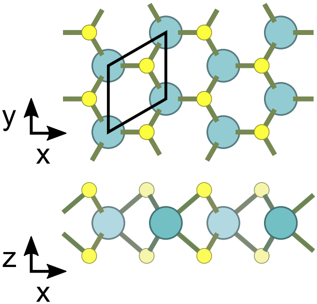
Compare: HgTe quatnum wells: **10-100 meV** (Bernevig et al. Science **314**, 1757 (2006))

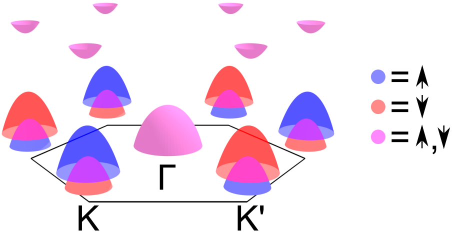
Are there any 2D materials with a large spin-orbit coupling?

Two-dimensional transition metal dichalcogenides

TMD = MX_2, $M = \{\textbf{Mo, W}\}$, $X = \{\textbf{S, Se, Te}\}$

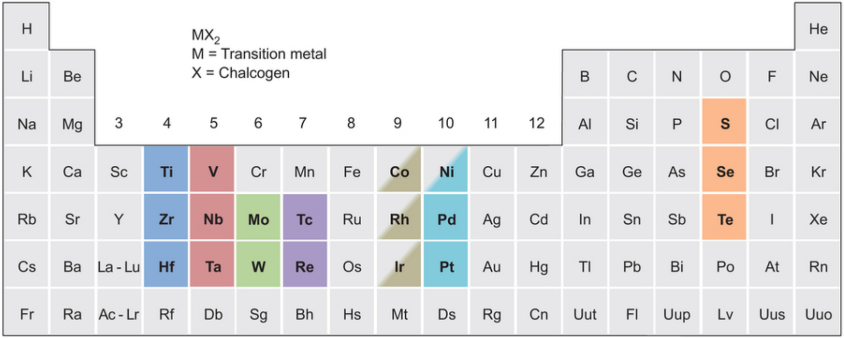
2H phase





- stable phase (except for $\mathrm{WTe_2}$), semiconductor in a hexagonal lattice;
- large spin-orbit splitting in the valence band (150 meV in $\mathrm{MoS_2}$, up to 460 meV in $\mathrm{WSe_2}$): spin-polarized states;
- spin-valley coupling

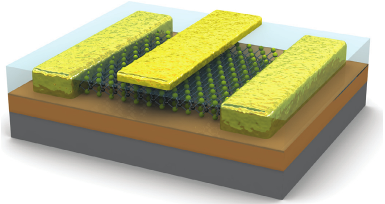
2D TMDs



M. Chhowalla, et al., Nat Chem **5**, 263275 (2013)

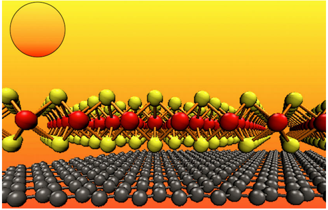
Applications

Transistors



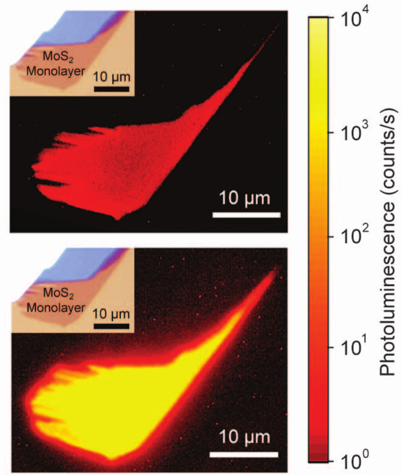
Radisavljevic et al., Nat Nano **6** no. 3 147-150 (2011)

Solar cells



Bernardi el al., Nano Lett. **13** no. 8 3664-3670 (2013)

LEDs

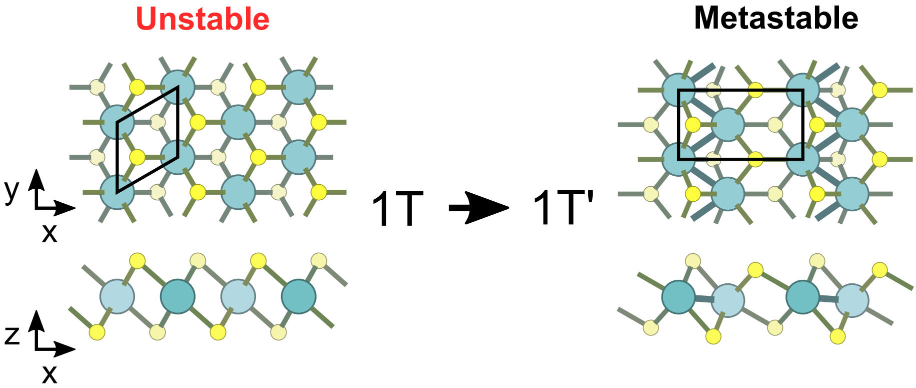


Amani et al., Science **350** no. 6264 1065-1068 (2015)

Is it possible to drive 2D TMDs into the **QSH phase**?

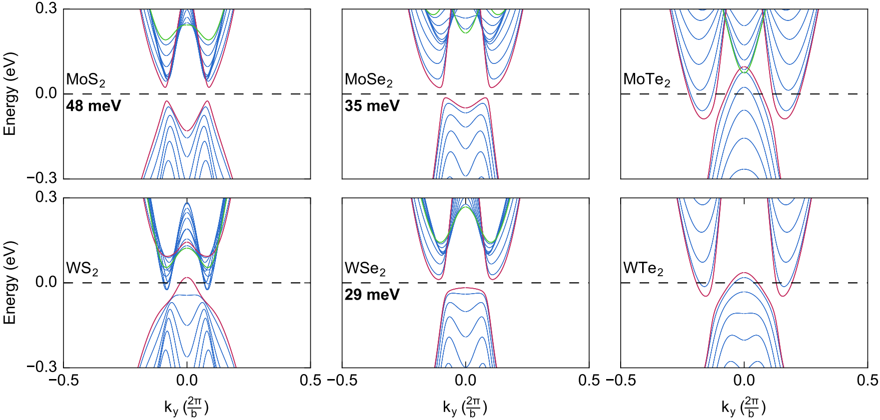
QSH effect in 2D TMDs

1T' phase



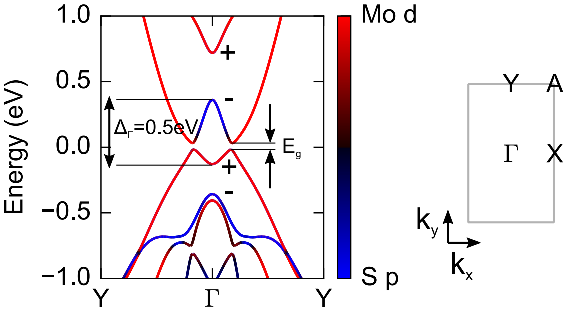
- same material in a metastable structure
- hexagonal symmetry breaking → rectangular unit cell
- formation of dimerization chains

Electronic properties of the 1T' structural phase



- spin-degenerate bands (inversion + time reversal symmetries)
- semimetals or semiconductors with a 10 meV-order band gap
- **topological band inversion**

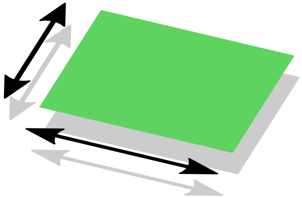
QSH phase in 1T' 2D TMDs



band inversion at Γ $\rightarrow$ quantum spin Hall (QSH) topological phase

Qian et al., Science **346**, 1344-1347 (2014)
Choe et al., Phys. Rev. B **93**, 125109 (2016)

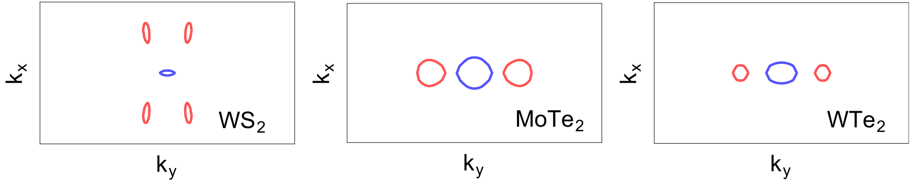
Is the QSH phase in 1T' TMDs robust against lattice deformations?



Electronic structure in equilibrium

At the density functional theory level (GGA):

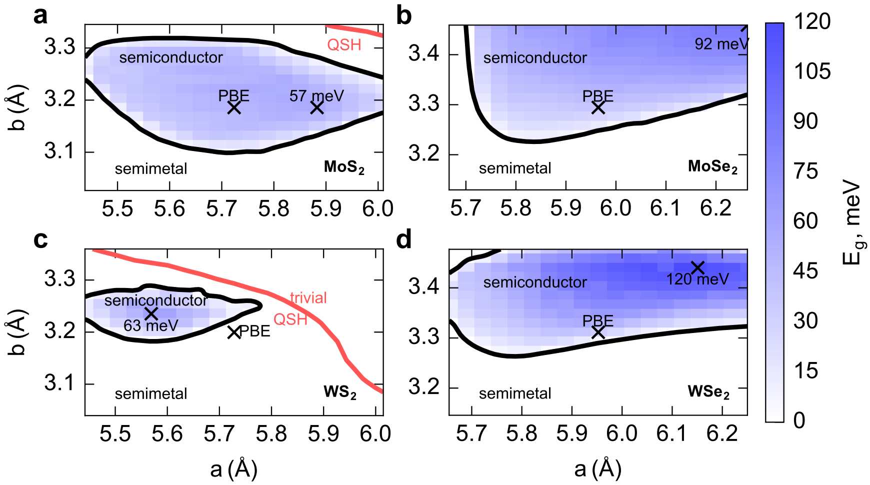
- MoS_2, $MoSe_2$, WSe_2 **have a band gap**;
- WS_2, $MoSe_2$, WTe_2 are **semimetals**;



Hole, electron pockets in semimetallic 1T' TMDs

Close to semiconducting phase transition phase?

Band gap under strain in 1T' 2D TMDs

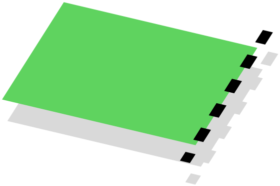


Pulkin & Yazyev Journal of Electron Spectroscopy and Related Phenomena **219** 72-76 (2017)

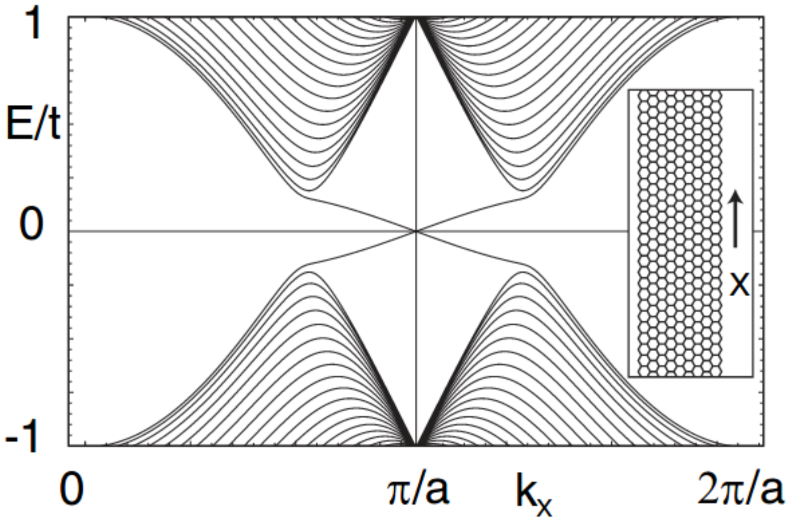
Conclusions

- 1T'-TMDs posess a **topological band inversion** at the Gamma point;
- $\mathrm{MoS_2}$, $\mathrm{MoSe_2}$, $\mathrm{WSe_2}$ also have a positive band gap $\rightarrow$ **topological insulators**;
- The size of the band gap is sensitive to lattice deformations;
- Both semiconductor-to-semimetal and topological phase transitions can be induced by strain

How do topological edge states in 1T' TMDs look like?

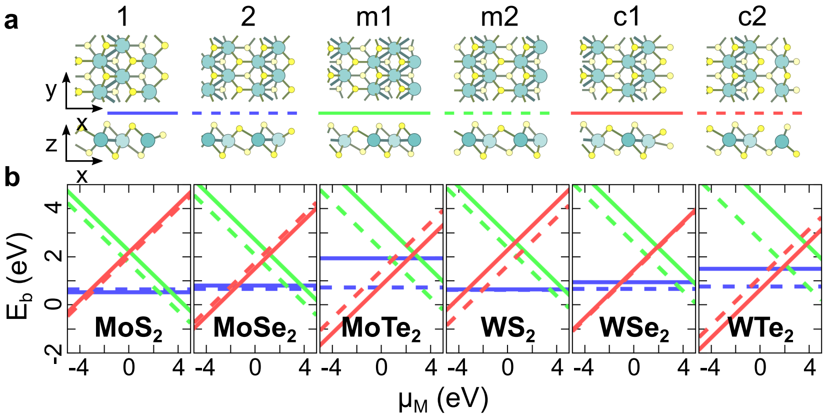


Recall: Kane-Mele model

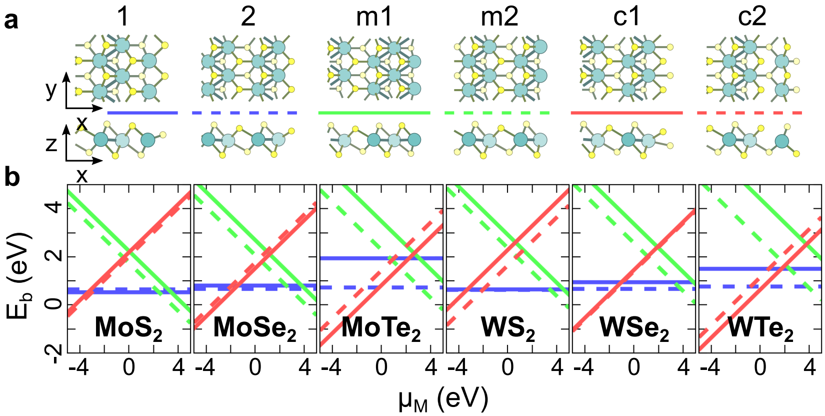


Edges in 1T' TMDs

- The "zigzag" edge



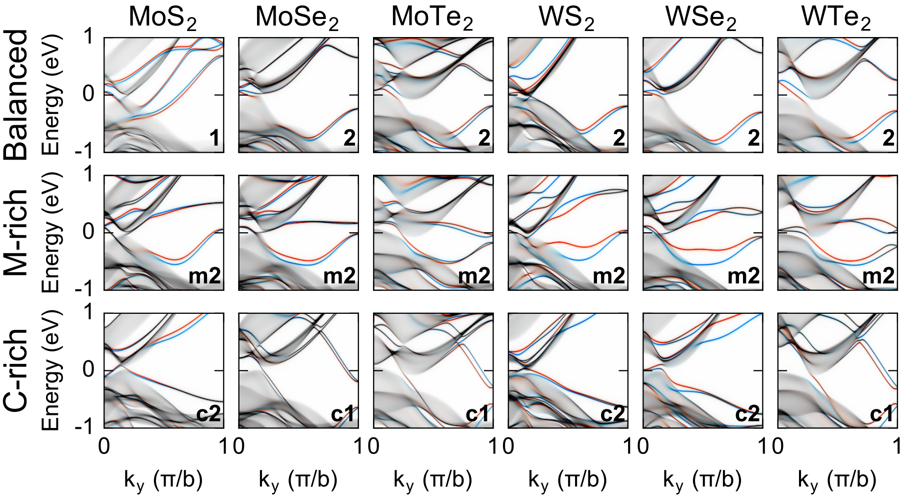
1,2 = neutral m1,m2 = metal-rich c1,c2 = chalcogen-rich



- **m2** is always preferred for metal-rich conditions;
- **2** is usually preferred for chemically balanced conditions;
- **c1**, **c2** are equally preferred for calcogen-rich conditions

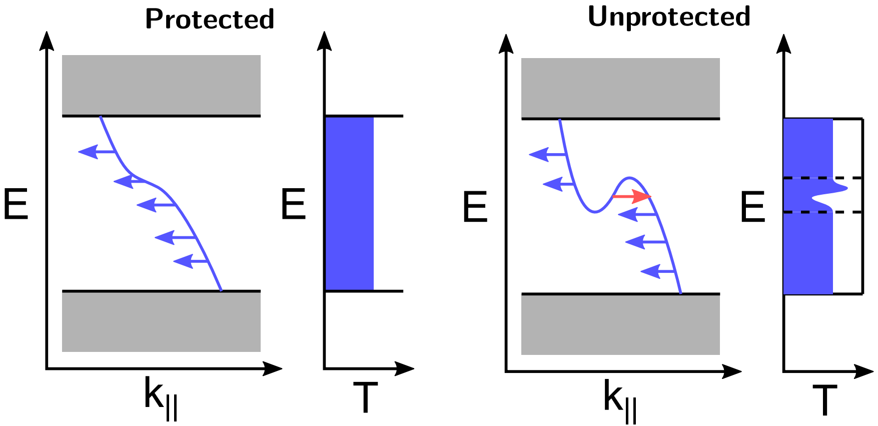
Electronic properties of edges in 1T' TMDs

- Energetically preferred terminations are considered;
- Method: DFT + Green's function (NEGF)



Is topological protection of the ballistic transport regime possible?

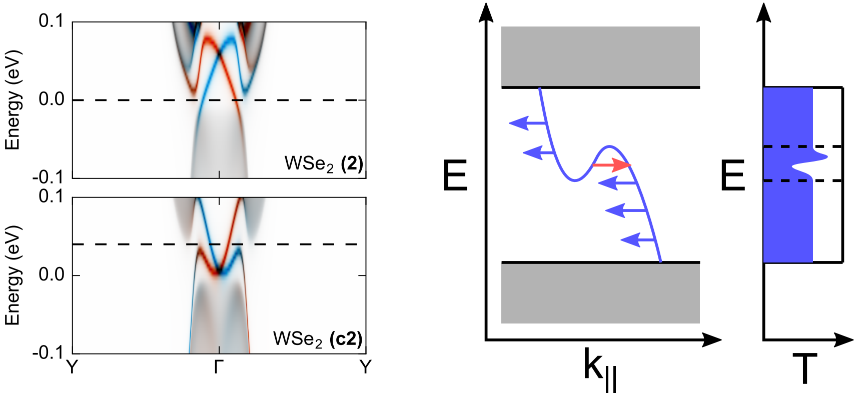
Topologically protected transport



topological protection $\neq$ protection against back-scattering

[0] A single spin channel is shown

Ballistic transport along 1T'-WSe_2 edges

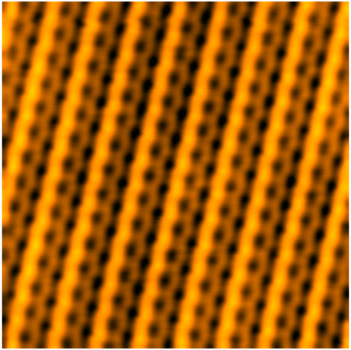


- non-uniform dispersion of edge modes;
- protected transport is **possible** in a narrow energy region and only at specific edges of 1T'-WSe_2

What is available experimentally?

Experimental observations of the 1T' phase in 2D WSe_2

✓ Defect-free bulk

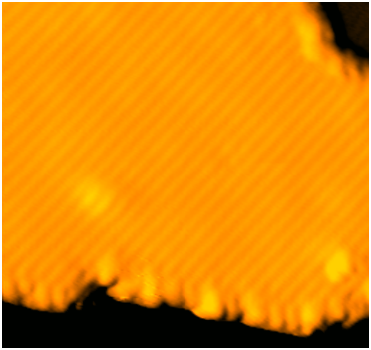


Images are courtesy of Miguel M. Ugeda, **nanoGUNE**, San Sebastian, Spain

Experimental observations of the 1T' phase in 2D WSe_2

✓ Defect-free bulk

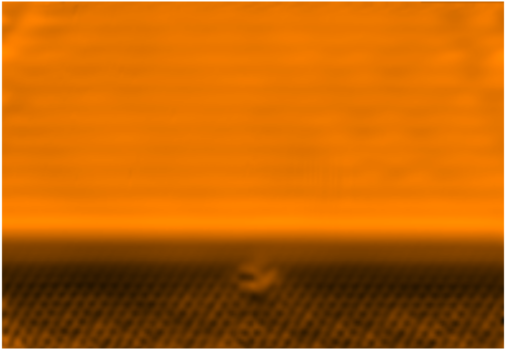
? Regular periodic edges



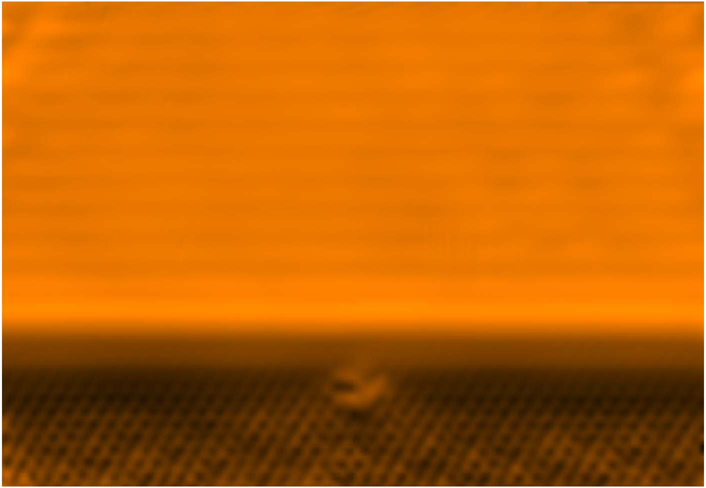
Images are courtesy of Miguel M. Ugeda, **nanoGUNE**, San Sebastian, Spain

Experimental observations of the 1T' phase in 2D WSe_2

- ✓ Defect-free bulk
- ? Regular periodic edges
- ! Structural phase boundaries

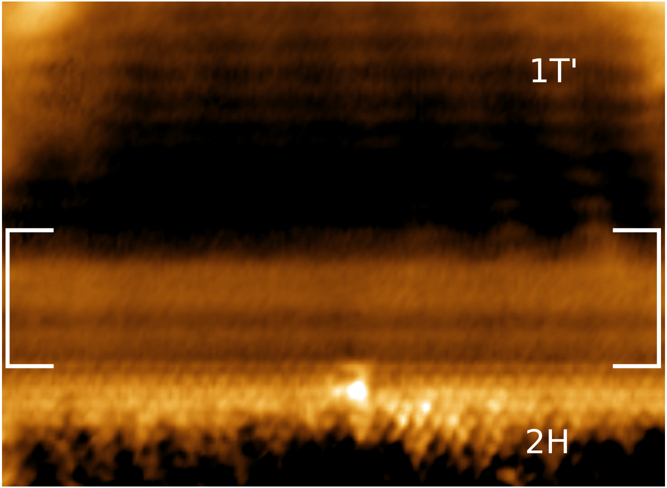


Images are courtesy of Miguel M. Ugeda, **nanoGUNE**, San Sebastian, Spain



Structural phase boundary is **topologically non-trivial**

1T'-WSe_2 interface states



Images are courtesy of Miguel M. Ugeda, **nanoGUNE**, San Sebastian, Spain

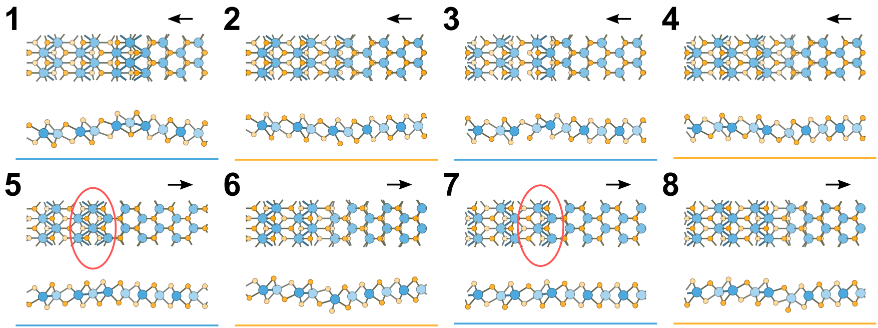
Can theory confirm the presence of interface modes?

Are these modes “topological”?

Atomic structures of phase boundaries in WSe_2

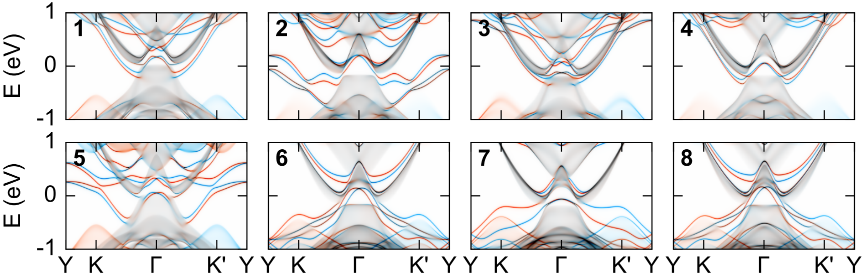
Construct model:

- choose the zigzag edge of the 2H phase (2x);
- choose the zigzag edge of the 1T' phase (4x, half discarded);
- concatenate



Electronic structure of phase boundaries in WSe_2

- Method: DFT + NEGF



- **1**, **3** and **6**, **8** are similar
- Multiple spectroscopic signatures
- No topological protection of transport

Conclusions

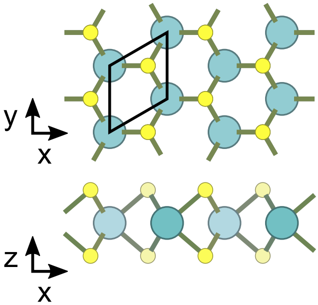
- Edge modes of real topological materials require *ab-initio* description;
- DFT+NEGF calculations reveal multiple spin-polarized modes spanning a large energy region in 1T'-TMDs;
- The dispersion of edge modes is consistent with the QSH phase;
- Specific 1T'-WSe_2 edges are suitable for ballistic charge carrier transport protected against back-scattering;
- **Regular topological phase boundary is accessible experimentally!**

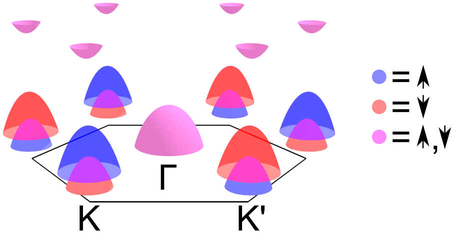
Topological edge states carry **spin-polarized current in a non-magnetic media** $\rightarrow$ applications for spintronics and quantum computing.

Other examples in 2D?

Idea

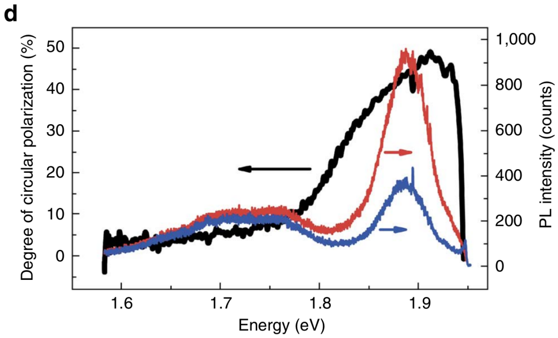
2H phase





Discriminate valleys in *some* physical process → spin-valley coupling → **induce spin polarization**

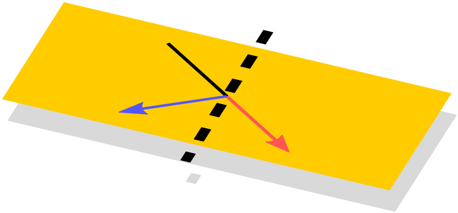
Example: optical excitation of charge carriers in semiconducting 2D MoS_2



Cao et al. Nat Commun **3** 887 (2012)

Also: Mak et al. Nat Nano **7** no. 8 494-498 (2012); Zeng et al., Nat Nano **7** no. 8 490-493 (2012)

Is it possible to achieve valley **polarization** in an **all-electric** manner?



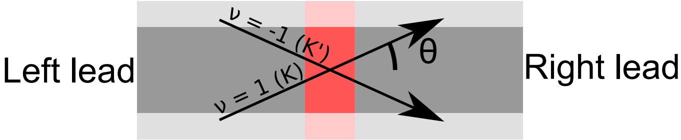
Idea: valley-polarized transport across a line defect

D. Gunlycke and C.T. White PRL **106**, 136806 (2011), *graphene*

- Symmetry: $T_{\nu}(\theta) = T_{-\nu}(-\theta) \neq T_{-\nu}(\theta)$,
- Polarization:

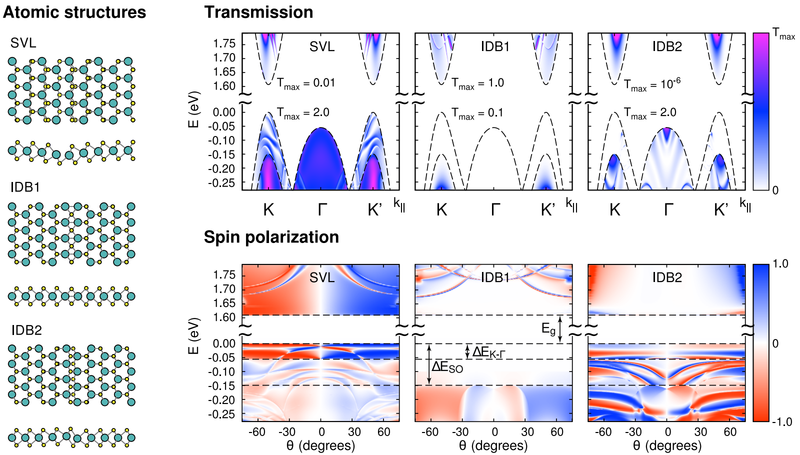
$$P(\theta) = \frac{T_{\nu=1} - T_{\nu=-1}}{T_{\nu=1} + T_{\nu=-1}} \approx \sin\theta$$

T_{ν} - transmission probability; $\nu = \pm 1$ - valley; θ - group velocity angle



In TMDs **valley ν and spin σ are coupled!**

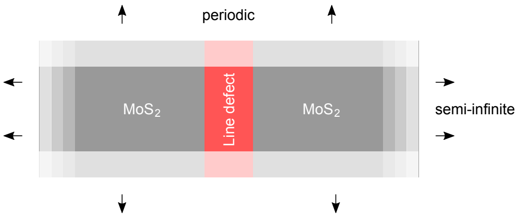
Pulkin & Yazyev, Phys. Rev. B **93** 041419(R) (2016)



- **valley and spin filtering** with strong energy dependence
- spin-orbit transport gap for holes in IDB1

Poor/no transport across inversion domain boundaries: why?

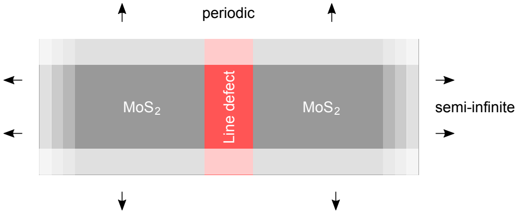
Ballistic transport



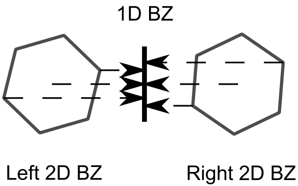
Take into account:

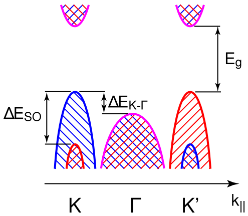
- conservation of **energy** (= ballistic transport);
- conservation of **pseudo-momentum** (= periodic line defect);
- conservation of **spin** (= planar non-magnetic defects)

Ballistic transport



Project the bands onto 1D Brillouin zone (BZ) of the defect (size $2\pi/\mathrm{d}$)



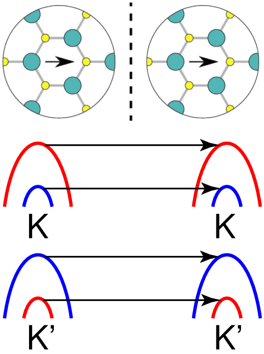


d - periodicity of the defect $\gtrsim$ a - TMD lattice constant (3-4 Å)

Transport gap $\mathrm{E_t}$

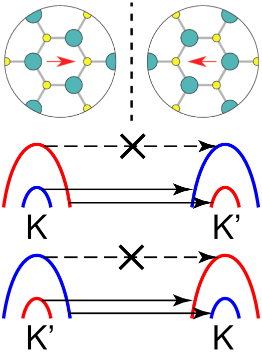
Spin match (no gap)

e.g. sulfur vacancy line



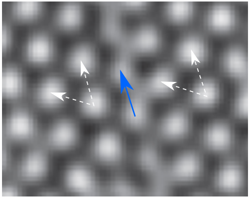
Spin mismatch (transport gap)

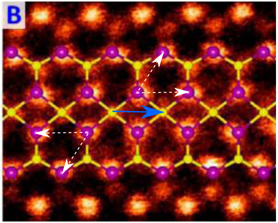
e.g. inversion domain boundary

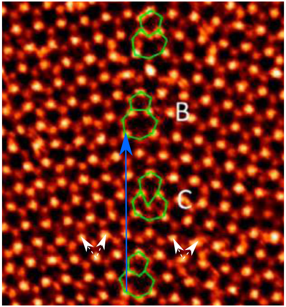


Transport gap $\mathrm{E_t}$: criterion

Other line defects with a transport gap?







Defect periodicity vector

$$\mathbf{d} = n_\mathrm{L}\mathbf{a}_{1,\mathrm{L}} + m_\mathrm{L}\mathbf{a}_{2,\mathrm{L}} = n_\mathrm{R}\mathbf{a}_{1,\mathrm{R}} + m_\mathrm{R}\mathbf{a}_{2,\mathrm{R}}$$

$$\mathbf{d} = (1,0) \quad |\mathbf{d}| = a = 0.3\ \mathrm{nm}$$

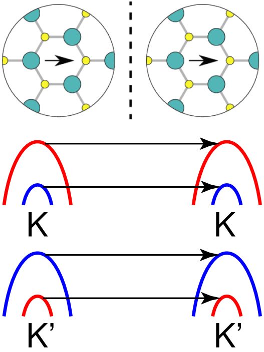
$$\mathbf{d} = (1,0)_\mathrm{L} = (-1,0)_\mathrm{R} \quad |\mathbf{d}| = a = 0.3\ \mathrm{nm}$$

$$\mathbf{d} = (3,5)_\mathrm{L} = (5,3)_\mathrm{R} \quad |\mathbf{d}| = 7a = 2.2\ \mathrm{nm}$$

Komsa et. al. PRB **88**, 035301 (2013); Zhou et. al. Nano Lett. **13**, 2615-2622 (2013)

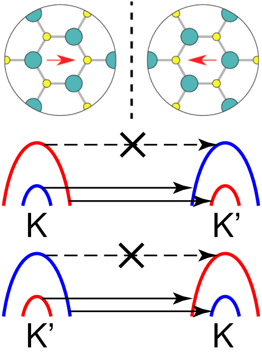
Transport gap E_t: criterion

Spin match (no gap)
e.g. sulfur vacancy line



$(n_L - m_L) \mod 3 = (n_R - m_R) \mod 3 \neq 0$

Spin mismatch (transport gap)
e.g. inversion domain boundary



$0 \neq (n_L - m_L) \mod 3 \neq (n_R - m_R) \mod 3 \neq 0$

Summary

- 2D TMDs are prospective materials for modern electronics, spintronics and topological electronic structure community;
- There is a large experimental effort towards confirming the **QSH phase in 1T'-TMDs**;
- Line defects found in these materials can be employed for **spin-selective transport** both along or across the defect, with or without relying on topological arguments;
- In either case, the spin polarization of charge carrier current exists **without net magnetization and macroscopic magnetic fields**: fewer spin relaxation channels and the increased spin lifetime in the material

Thank you