Center for Nanostructured Graphene

GRAPHENE FLAGSHIP

DTU

2D materials for Quantum Technology

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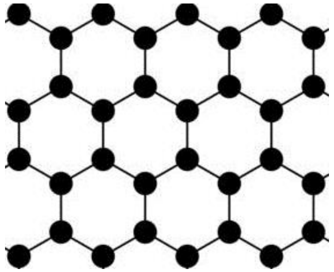
Technical University of Denmark

Outline: 2D Materials for Quantum Technologies

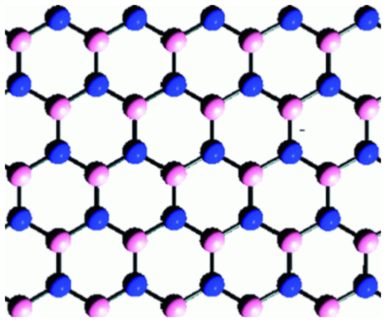
- Background: Qubits in conventional semiconductors

- Graphene* ⟶ Devices:
  - Spin Qubit *
  - Valley Qubit
  - Superconducting / Topol.protected
  - Plasmons

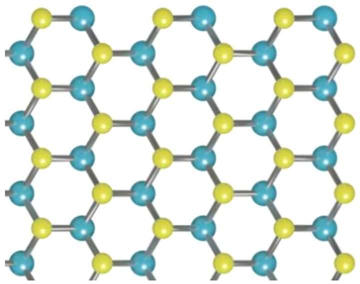


- C

- Other 2D materials (hBN, WSe2)



- N
- B



- W
- Se

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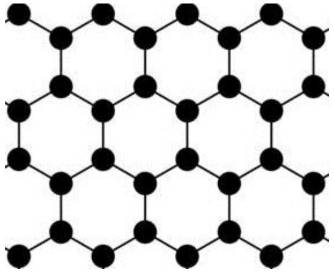

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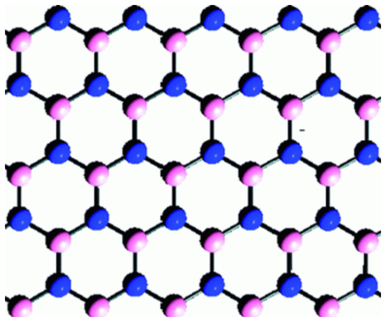

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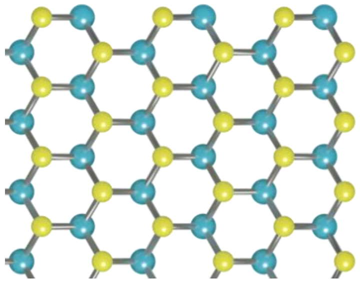

- W
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Qubits in conventional semiconductors

- Qubits: quantum analogue to the classical bit

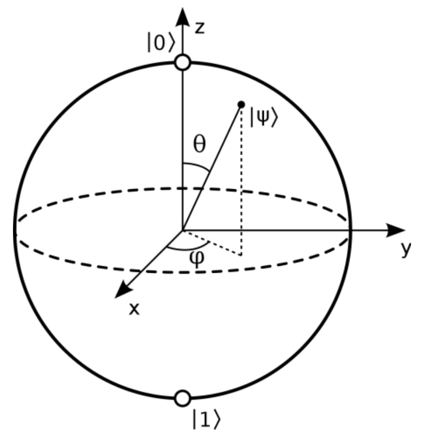
- Created based on any quantum two-level system (with coherent control)

Basis $|0\rangle$, $|1\rangle$

Quantum state:

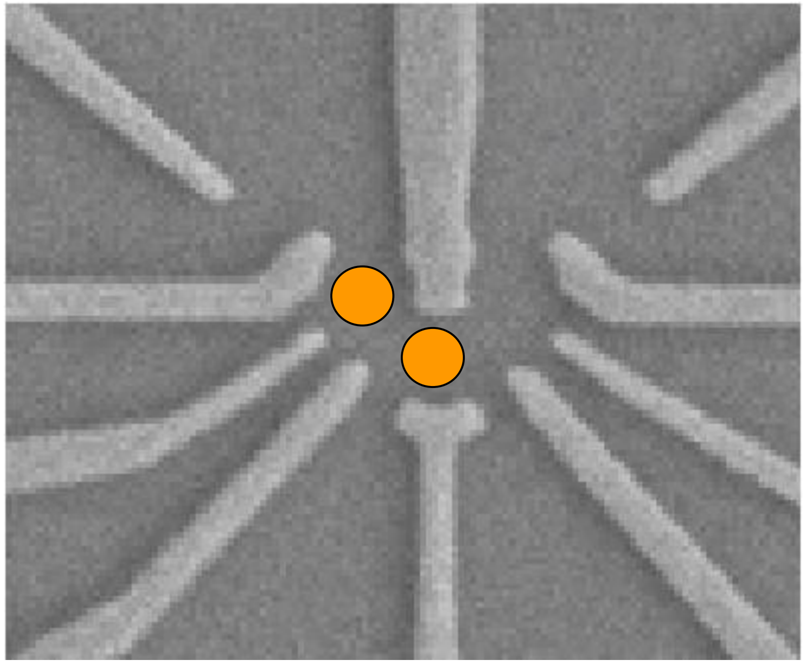
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Bloch sphere:



Qubits in conventional semiconductors

- First Qutbit demonstrations in quantum-dots in 2DEGs

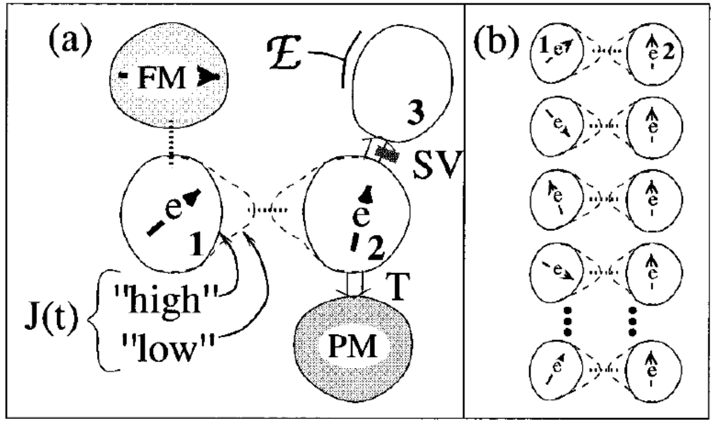


PHYSICAL REVIEW A VOLUME 57, NUMBER 1 JANUARY 1998

Quantum computation with quantum dots

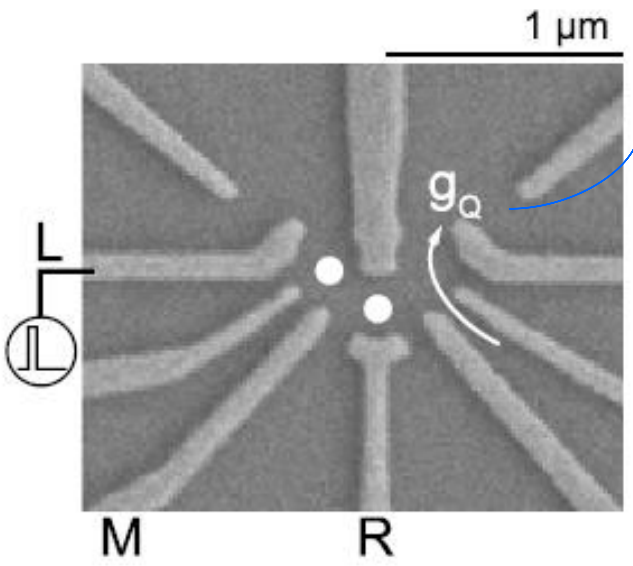
Daniel Loss[1,2,*] and David P. DiVincenzo[1,3,†]
[1]*Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, California 93106-4030*
[2]*Department of Physics and Astronomy, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland*
[3]*IBM Research Division, T.J. Watson Research Center, P.O. Box 218, Yorktown Heights, New York 10598*
(Received 9 January 1997; revised manuscript received 22 July 1997)

We propose an implementation of a universal set of one- and two-quantum-bit gates for quantum computation using the spin states of coupled single-electron quantum dots. Desired operations are effected by the gating of the tunneling barrier between neighboring dots. Several measures of the gate quality are computed within a recently derived spin master equation incorporating decoherence caused by a prototypical magnetic environment. Dot-array experiments that would provide an initial demonstration of the desired nonequilibrium spin dynamics are proposed. [S1050-2947(98)04501-6]

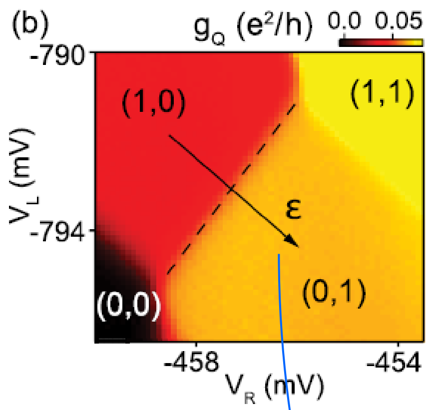


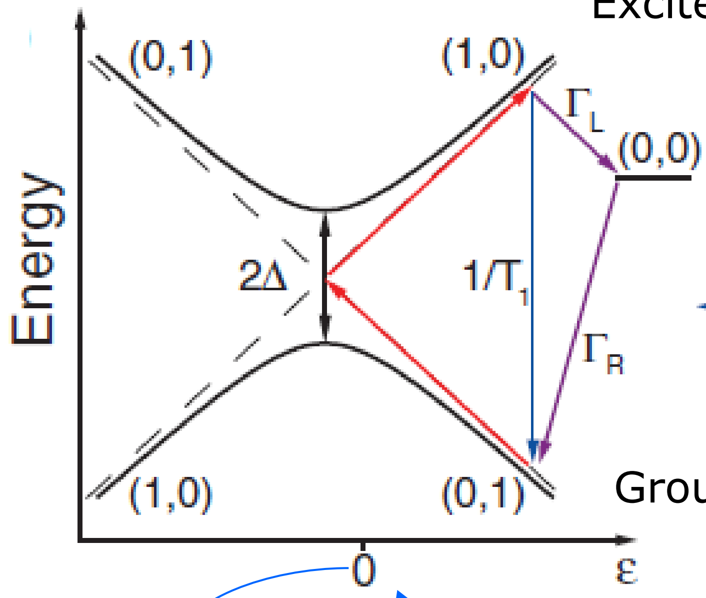
Qubits in conventional semiconductors

- Charge Qubit: "Position of single electron in left or rigth Qdot" basis $|L\rangle = (1,0)$ and $|R\rangle = (0,1)$



Charge detector (quantum point contact) with conductance g_Q





Interdot tunnel coupling 2Δ

(controlled by voltage V_M)

Detuning axis ε

"Oscillation between states"

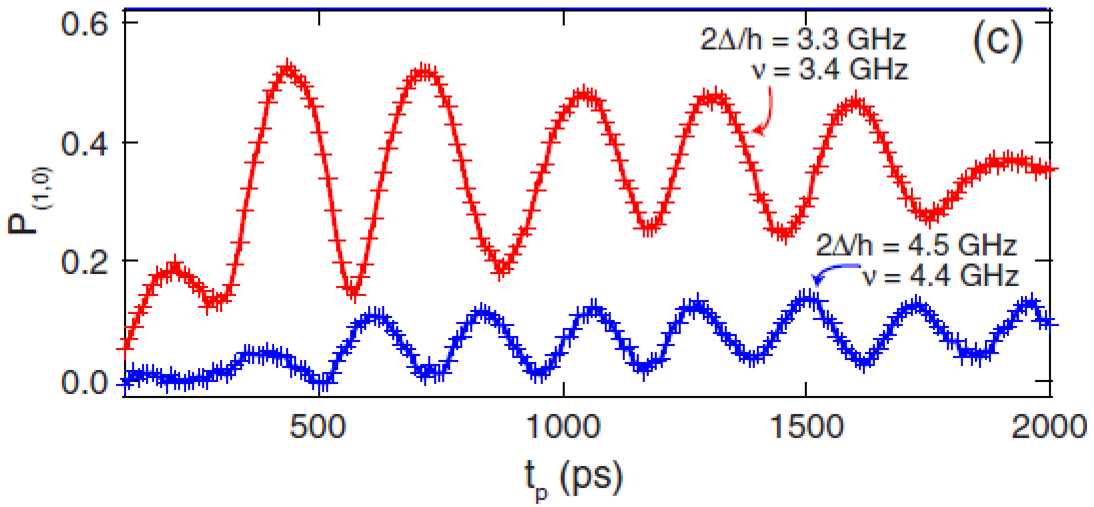
K.Petersson et al, PRL, 2010

Qubits in conventional semiconductors

• Charge Qubit: ”Position of single electron in left or rigth Qdot” basis $|L\rangle = (1,0)$ and $|R\rangle = (0,1)$

Oscillations at charge degeneracy point ε =0, for two tunnelling couplings *2Δ*

Left dot occupation



* Operation time (rotation quBit) ~100 ps

* Decoherence time ~ 2ns!!

K.Petersson et al, PRL, 2010

Qubits in conventional semiconductors

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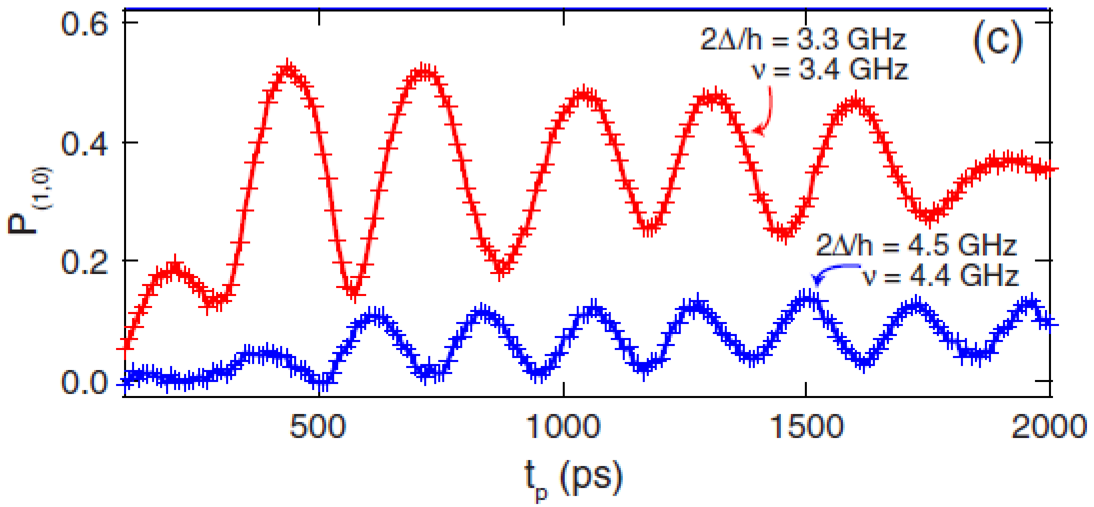


* Operation time (rotation spin) ~100 ps
* Decoherence time ~ 2ns!!
* Only 20 rotations!

(charge noise in the environment)

K.Petersson et al, PRL, 2010

Qubits in conventional semiconductors

- Spin Qubit:

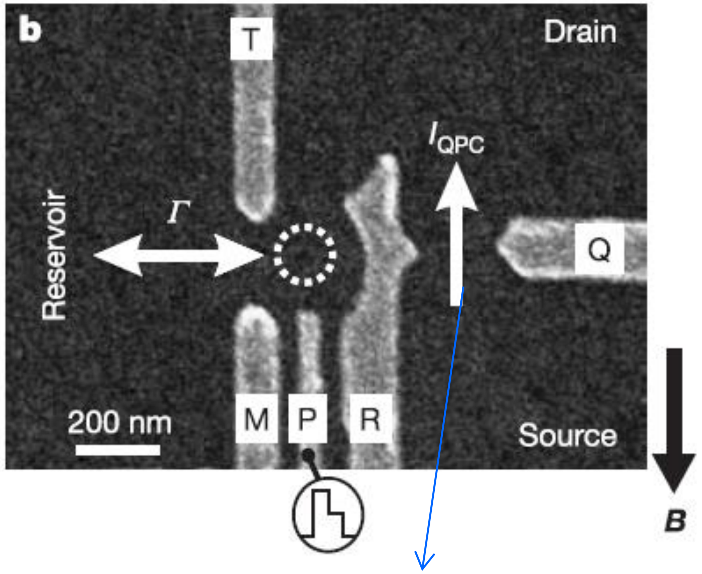
  - Spin degree of freedom in electrons is a quantum two-level system (basis ”spin-up”, ”spin-down”)

  - Electron spin is less coupled to environment than charge

  - Spin decoherence maninly only due to *i)* spin-orbit coupling SOC and *ii)* electron-phonon coupling EPC to lattice vibrations (all material parameters)

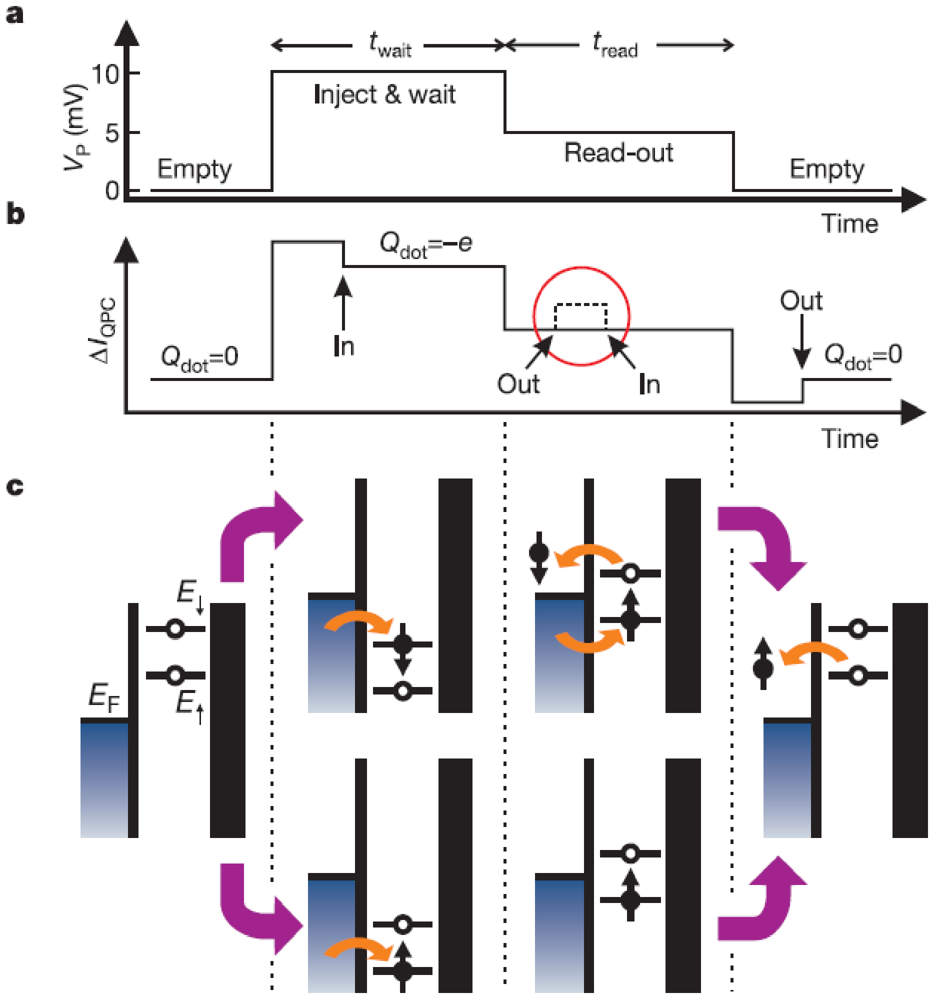
Qubits in conventional semiconductors

- Spin Qubit: Spin-read out



QPC Read-out (spin to charge conversion)

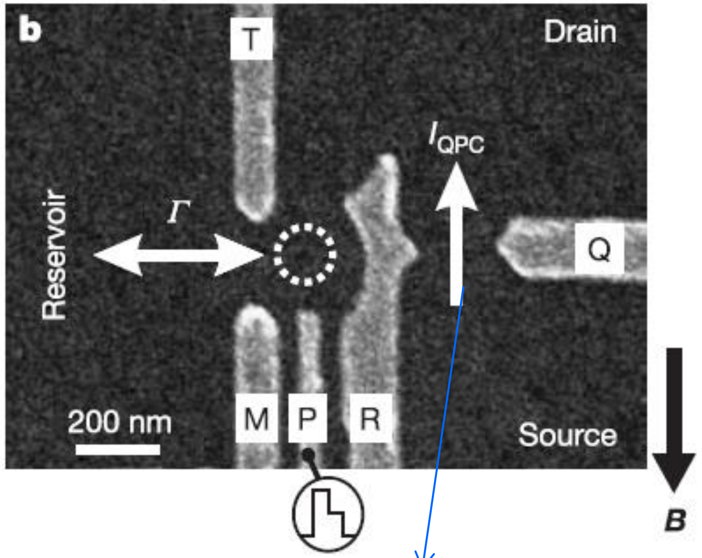
J.M. Elzerman et al. Nature (2004)



Qubits in conventional semiconductors

• Spin Qubit: Spin-read out

Experiments



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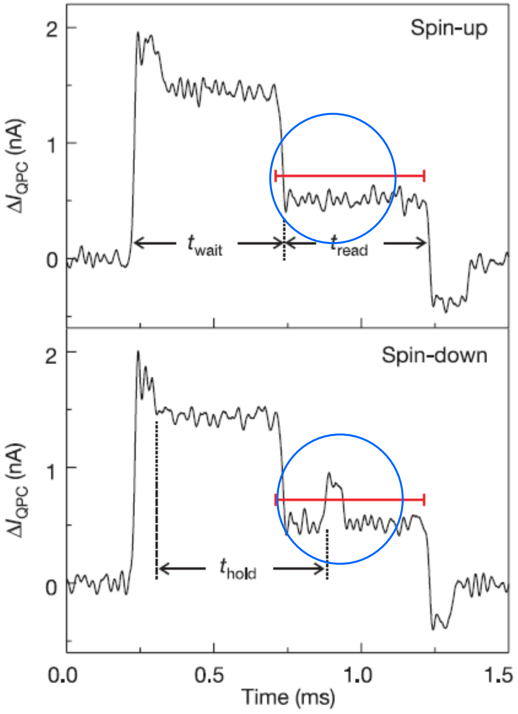

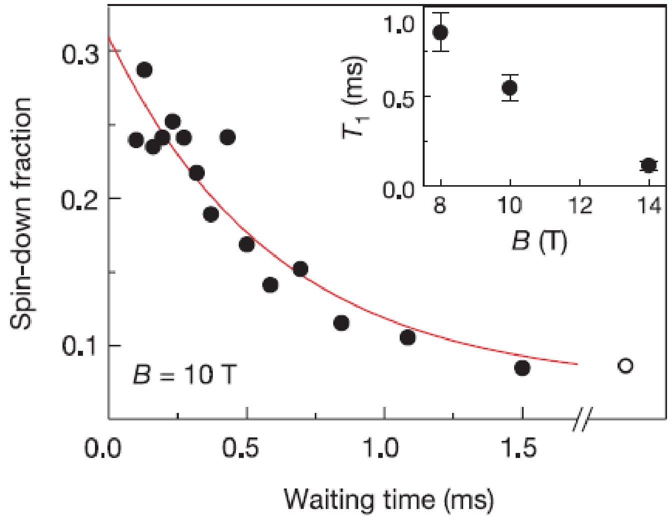

* Decoherence time > 1ms!!

J.M. Elzerman et al. Nature (2004)

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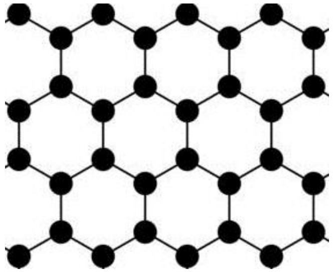

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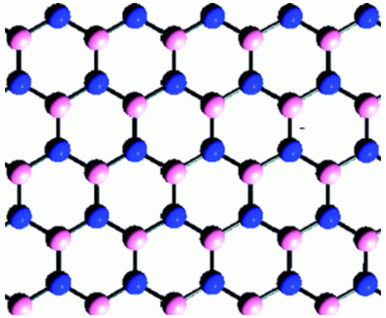
- Other 2D materials (hBN, WSe2)



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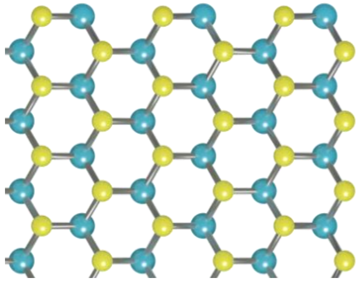
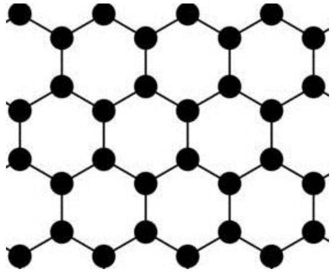


- W
- Se

Spin Qubits in graphene



• C

- Why Graphene / Graphene quantum dots?

  - Operation time (rotation of spin) 5 times faster

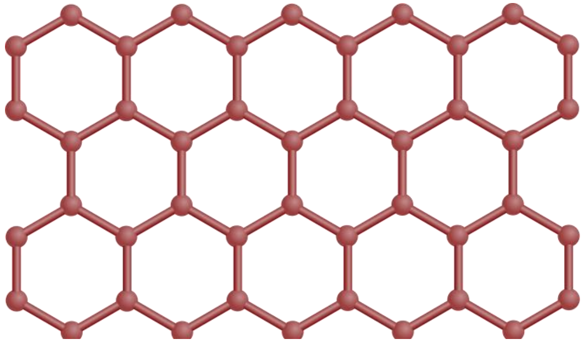
$$f_{\mathrm{Rabi}} = g\mu_B B_{ac}/2h$$

  - $|g|$ (GeAs) = 0.43
  - $|g|$ (graphene) = 2

  - Decoherence time is longer (low SOC in carbon, low EPC in graphene…)
  - Long distance Qubit coupling (due to Klein tunneling). Ideal for fault tolerant quantum computation
  - Further Qubit implementations (Valley Qbit, topologically-protected states, plasmons…)

Graphene lattice

Graphene:



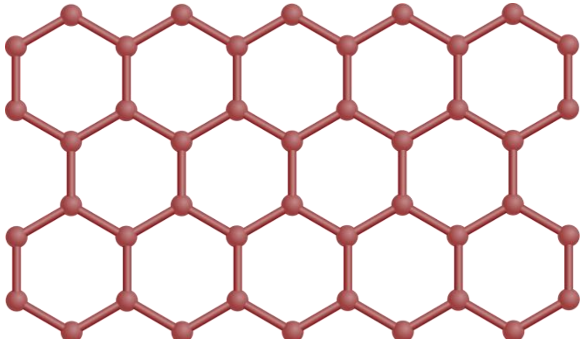
sp^2 hybridized Carbon →

honeycomb structure

C [$1s^2$, $2s^2$, $2p^2$]

Graphene lattice

Graphene:



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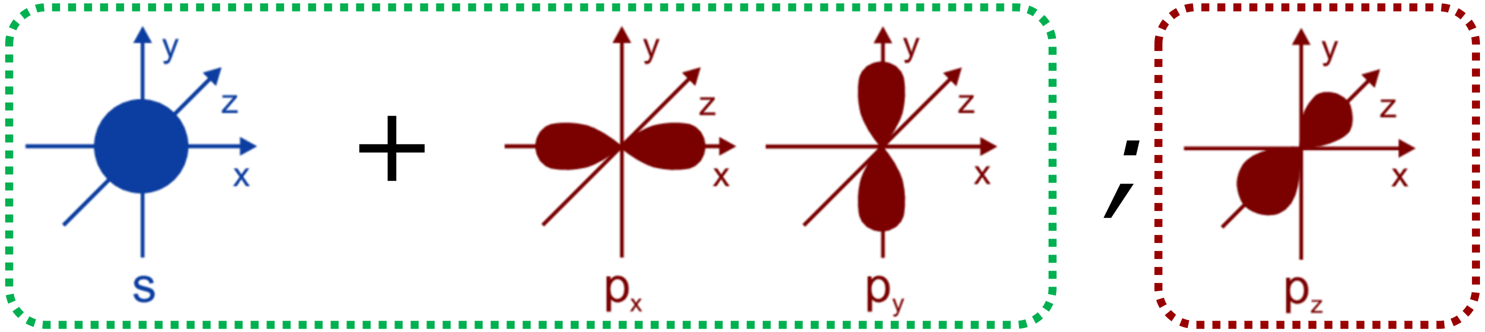
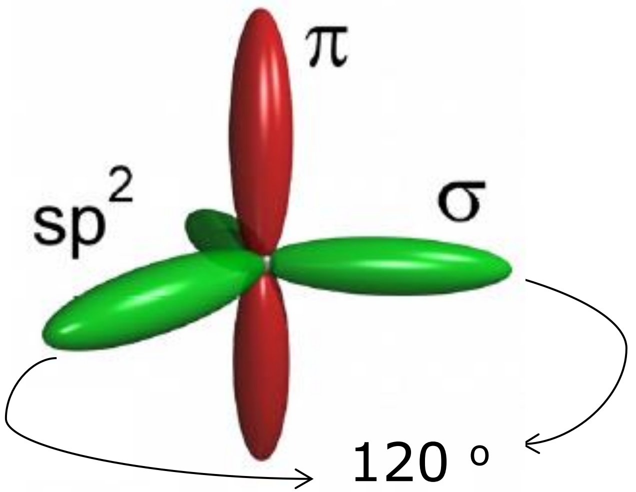
C – C bonds: sp^2

Atomic orbitals



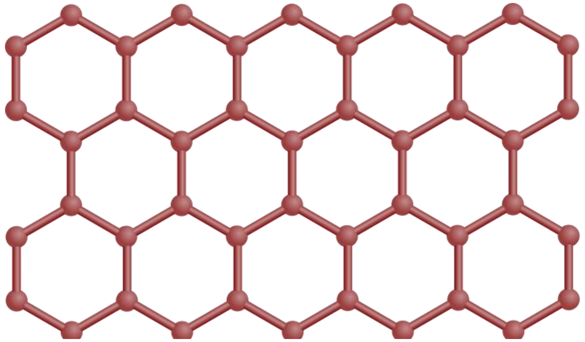
Hybridized molecular orbitals



4 orbitals, 3 hybridized (sigma-bonds), 1 unhybridized (pi –bonds)

Graphene lattice

Graphene:



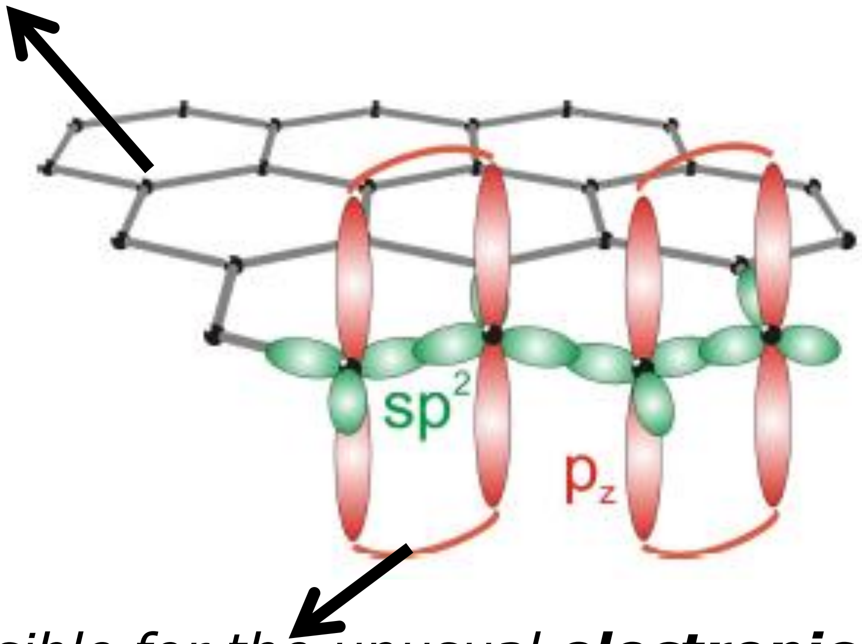
sp^2 hybridized Carbon →

hexagonal structure

C [$1s^2$, $2s^2$, $2p^2$]

Honeycomb structure

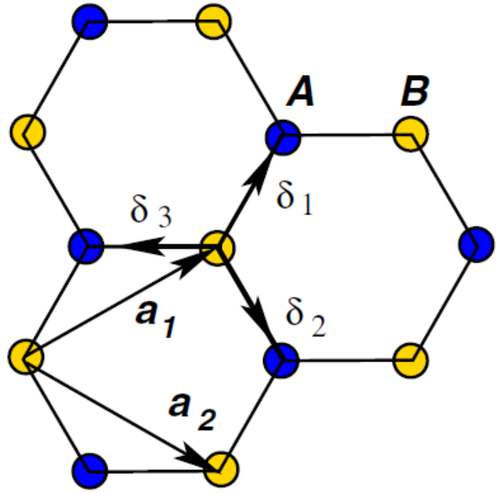
***Sigma –bonds** (sp2 orbitals), constitute the hexagonal structure and determine the **mechanical properties** of this 2D material*



***Π -bonds→** responsible for the unusual **electronic properties** of graphene*

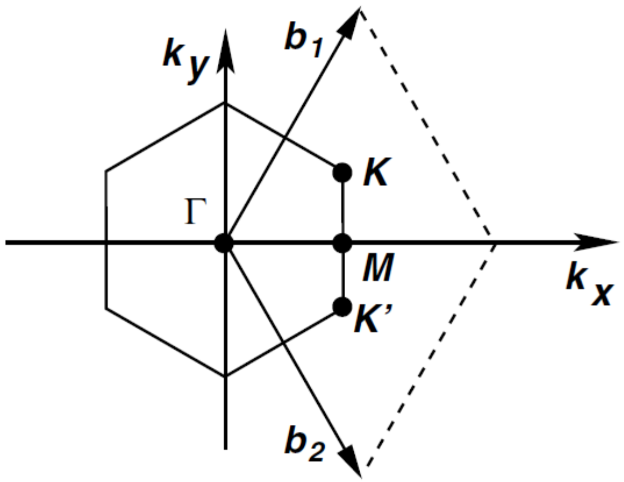
Electronic properties of graphene

Bandstructure: "Interaction of pi - electrons with hexagonal lattice"



Bravais lattice:
Triangular, with two identical atoms per unit cell

A ***B***

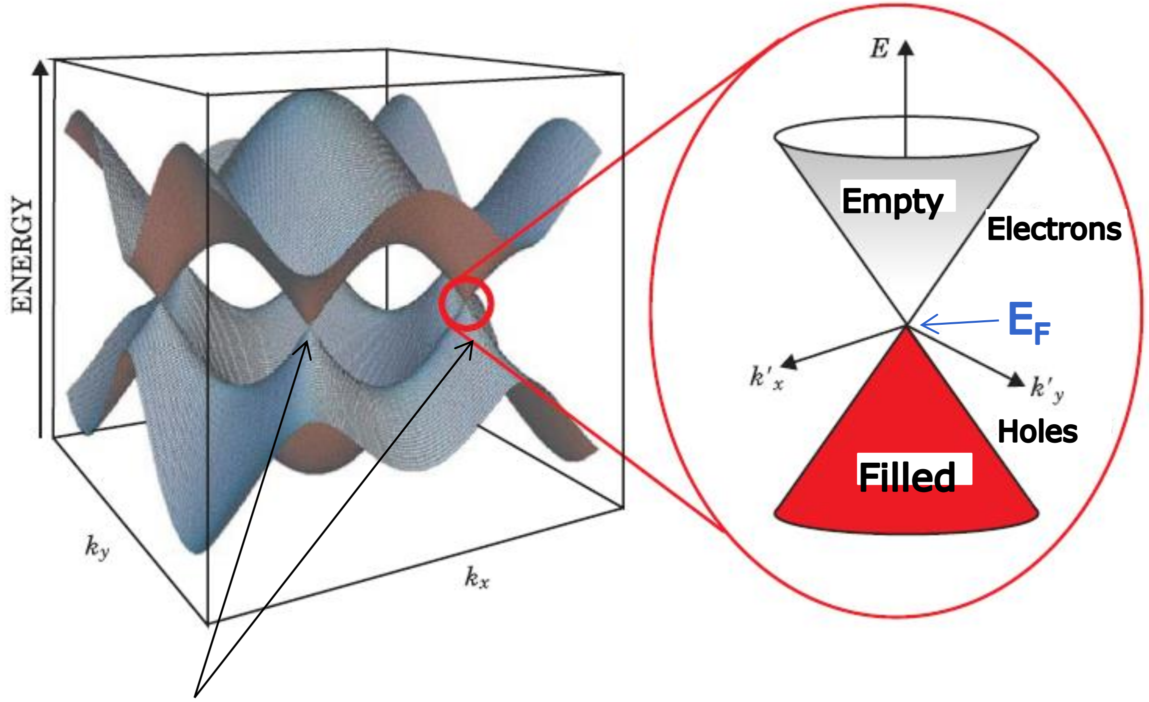


Brillouin zone:

K, **K'** are inequivalent corners

"Dirac points",

"valleys"



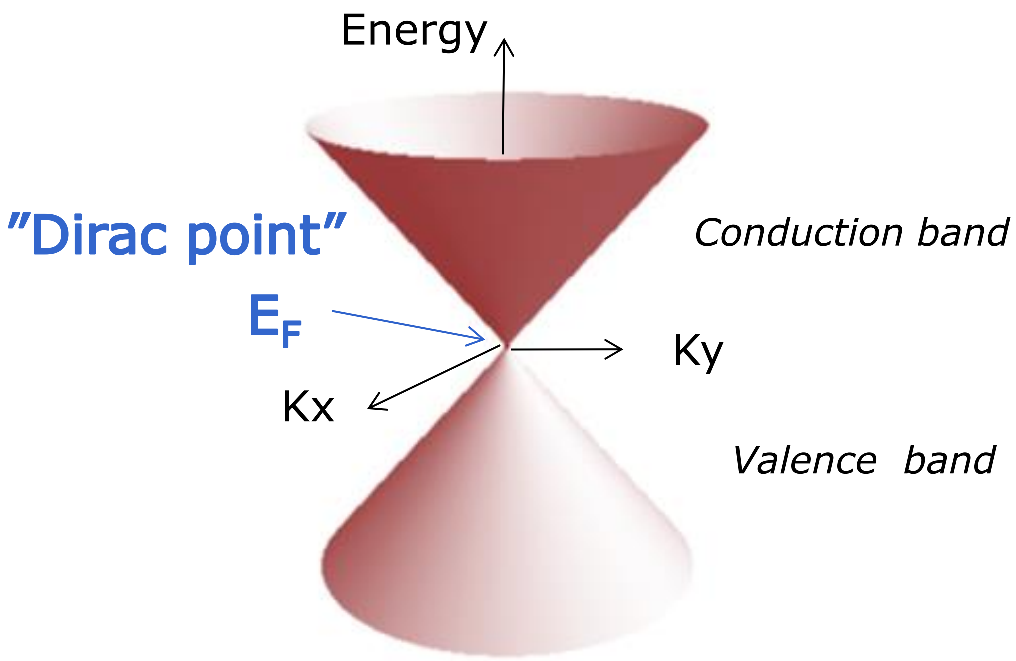
K', K

Das Sarma, et al. Rev. Mod. Phys, 83, 2011

Electronic properties of graphene

Linear Bandstructure:

$$E_{\pm}(q) = \pm \hbar v_F q$$



Unique Features (i)

- Relativistic charge carriers ($v_F \sim c/300$, zero mass)
- No band-gap (PROBLEM, NO QUANTUM DOTS BY ELECTROSTATIC CONFINEMENT due to relativistic tunneling!)

Das Sarma, et al. Rev. Mod. Phys, 83, 2011

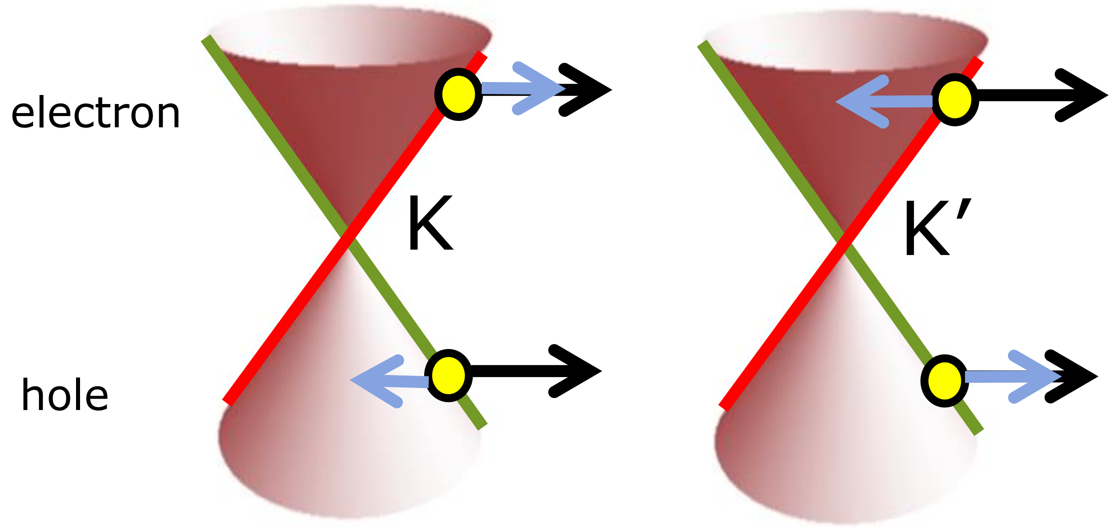
Electronic properties of graphene

Unique Features (ii)

Two component!!

- Two independent sublattices **A**,**B** (K, K′)
  - Crystal basis: **|A>** , **|B>**
  - Electron wavefunction: superposition **|A>** + $e^{i\theta}$ **|B>**
  - Phase θ, Pseudo-spin or valley degree of freedom

- Pseudo-spin is linked to the momentum (parallel or anti-parallel)
  - *momentum*
  - *pseudo-spin*



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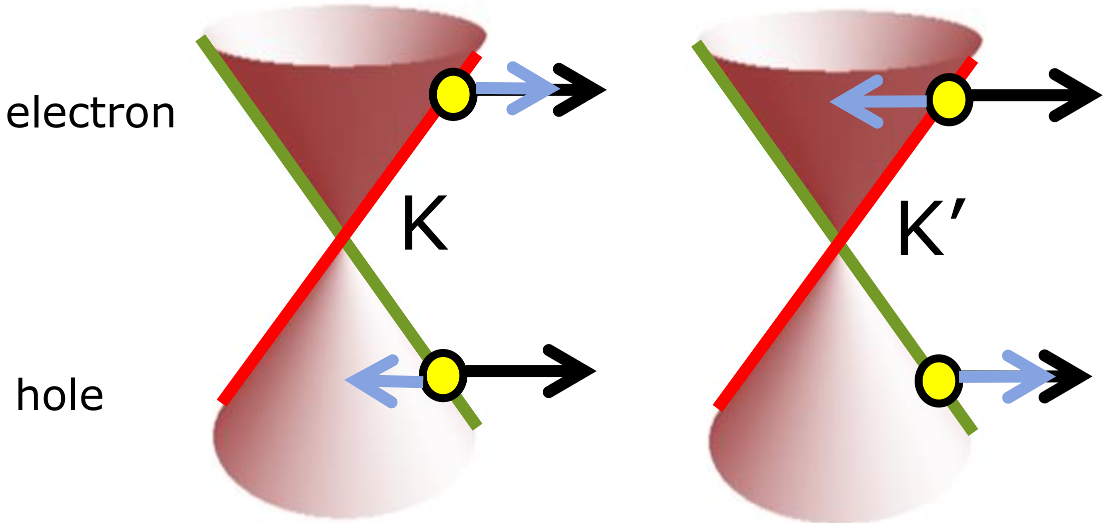

NEW (VALLEY) DEGREE OF FREEDOM,

Is it good or bad to create QuBits???

Das Sarma, et al. Rev. Mod. Phys, 83, 2011

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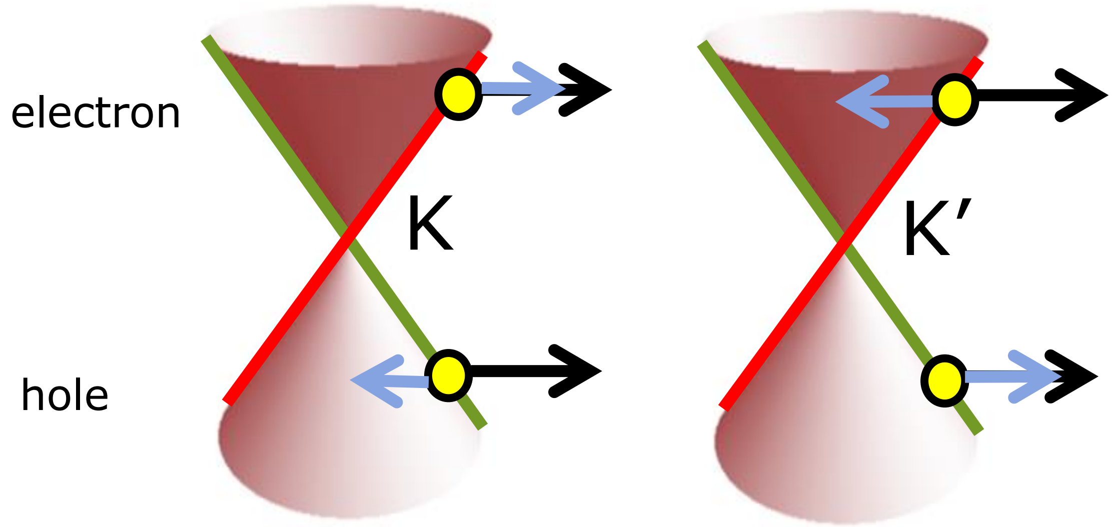


NEW (VALLEY) DEGREE OF FREEDOM,

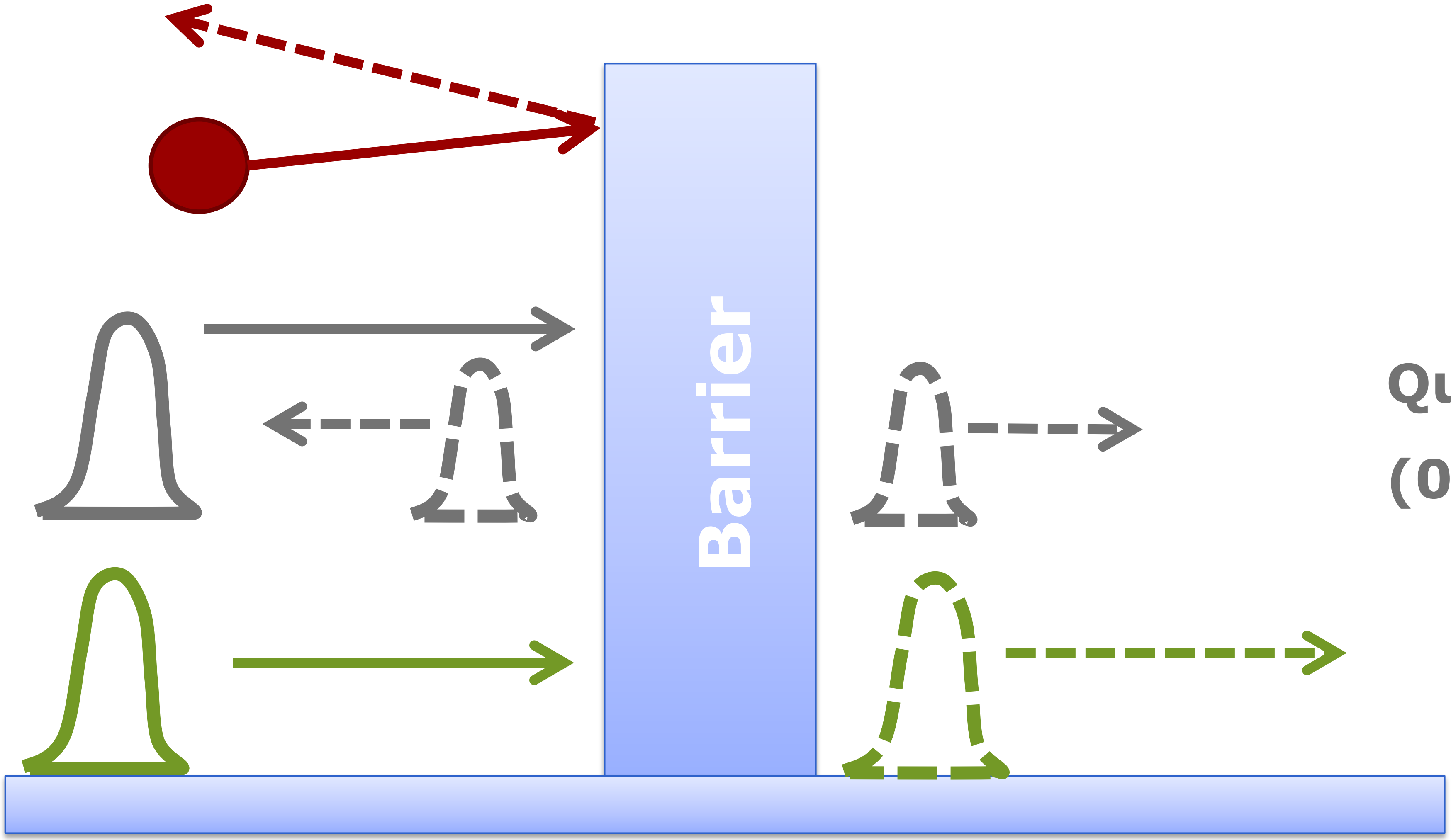
Is it good or bad to create QuBits???

- Advantages: Valley Qubits
- Disadvantages: valley degeneracy has to be lifted for spin Qubits - we need distinguishable states (spin, valley)

Das Sarma, et al. Rev. Mod. Phys, 83, 2011

Unique transport properties of graphene

- **Relativistic (Klein) tunneling** in graphene



Classial physics

(T=0)

Quantum mechanics

(0<T<1)

Quantum ED

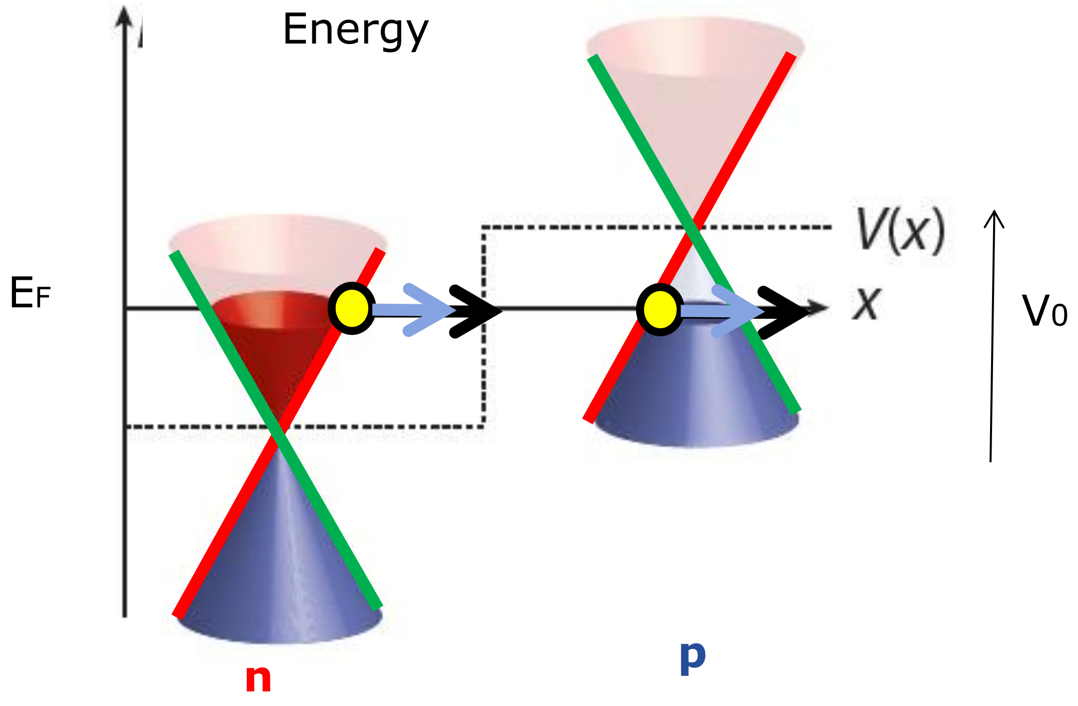
(T=1) "KLEIN PARADOX"

Katsnelson et al. Nat. Physics, 2006

Unique transport properties of graphene

- **Relativistic (Klein) tunneling** in graphene: **TRANSMISSION VIA NEGATIVE ENERGY STATES**

Realizable in graphene in SHARP pn (np) junctions



Graphene pn junction

- No pseudo-spin flip possible with an electrostatic potential V(x)
- Transmission =1

Katsnelson et al. Nat. Physics, 2006

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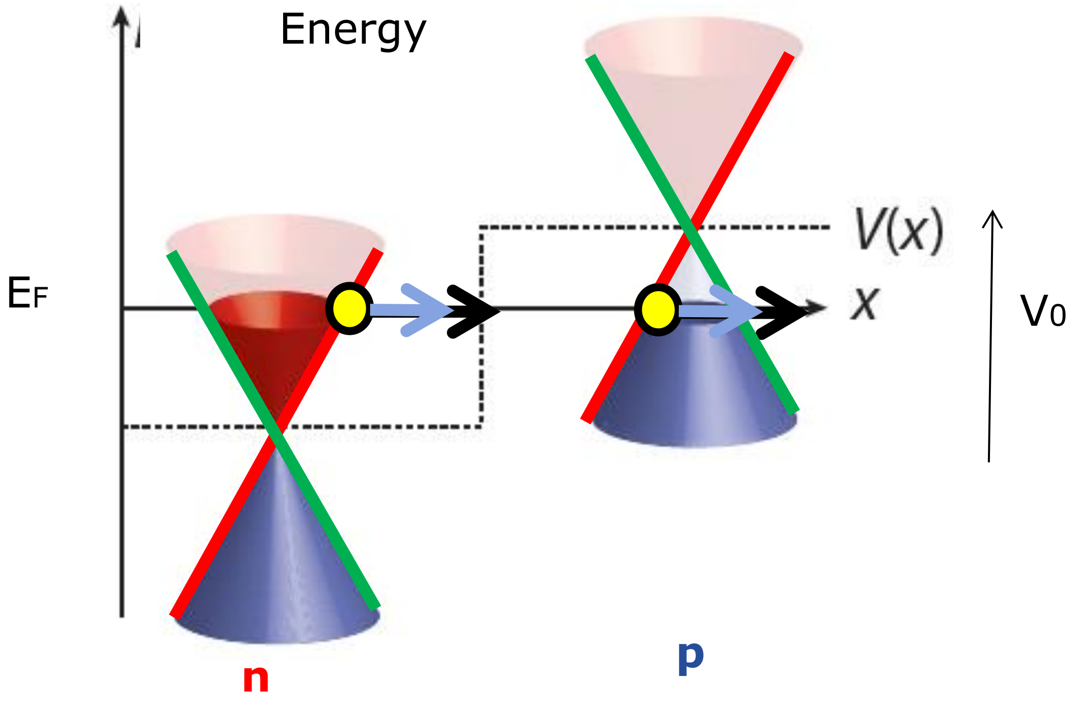

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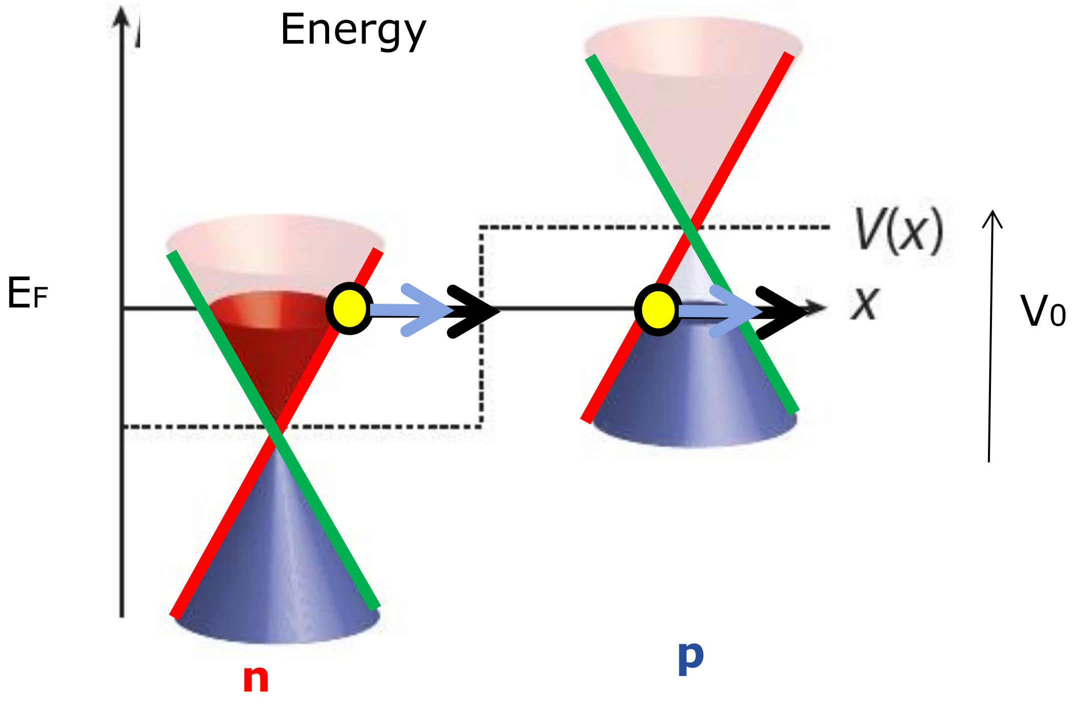

Graphene pn junction

KLEIN TUNNELING,

Is it good or bad to create QuBits???

- Disadvantages: no electrostatic confinement
  → No graphene quantum dots

- Advantages: Long distance QuBit coupling

Katsnelson et al. Nat. Physics, 2006

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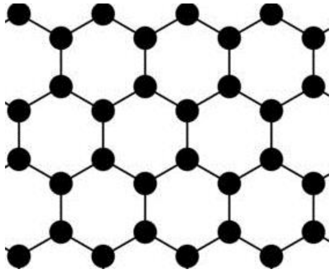

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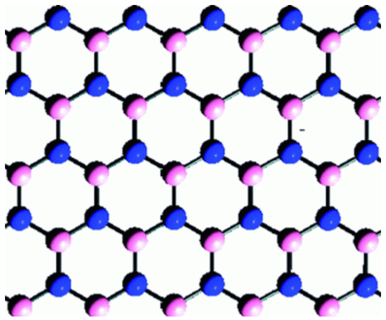

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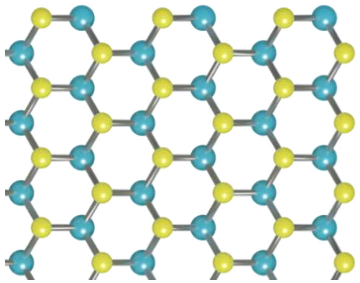
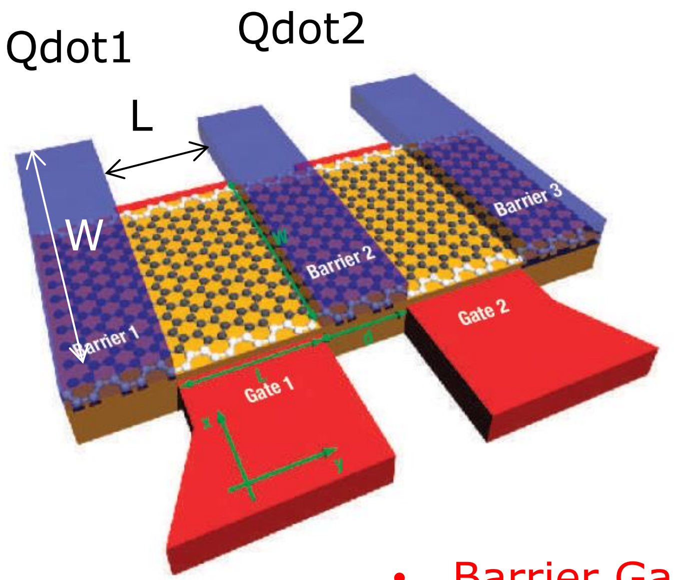


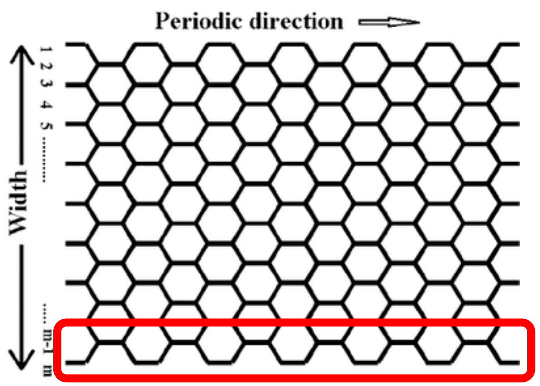
- W
- Se

Spin Qubits in graphene

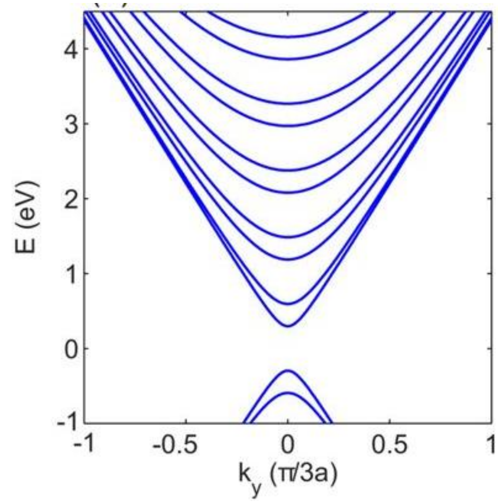
- **Predicted design: electrostatically confined graphene nanoribbons with armchair border**

RIBBONS WITH ARMCHAIR TERMINATION





- Induces a band-gap in graphene
- Valley degeneracy is lifted



- Barrier Gates (blue) → creation of quantum dot (size L x W) by electrostatic confinement.
- Barrier 2 (middle) creates a tuneable exchange coupling J between electron spins in left and right dot $H = JS_1S_2$
- Additional Gates (red)→ Tune the Fermi level of the dot

Trauzettel et al. Nat. Physics, 2007

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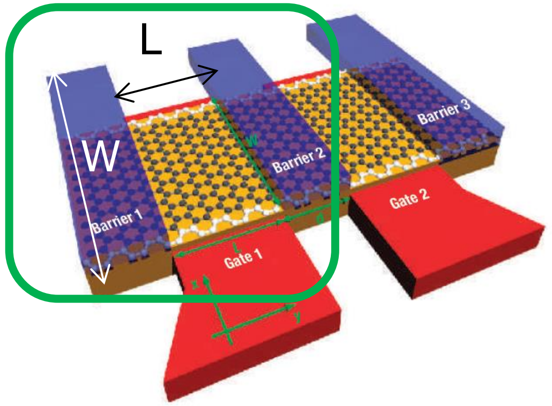
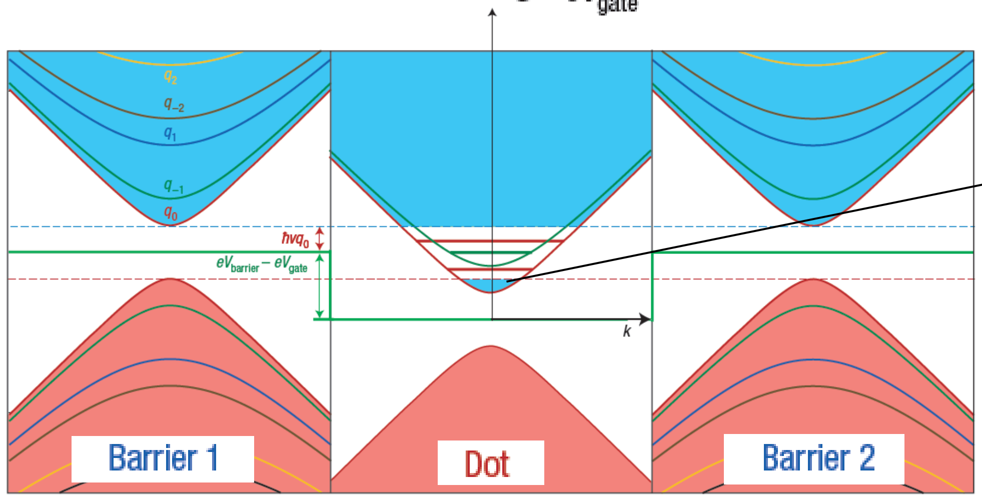
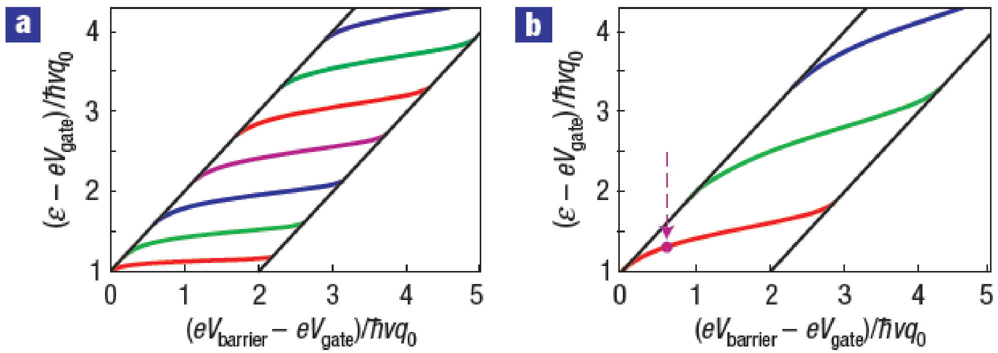


SINGLE DOT

Bound state solutions for single dots with two diffent lenghts (L1>L2)



L1 L2

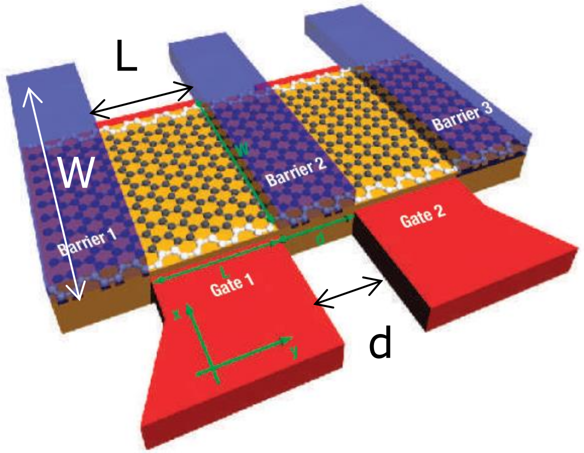


Level spacing $\Delta\varepsilon \approx \hbar v \pi / \max\{W, L\}$ ~10 meV

Trauzettel et al. Nat. Physics, 2007

Spin Qubits in graphene

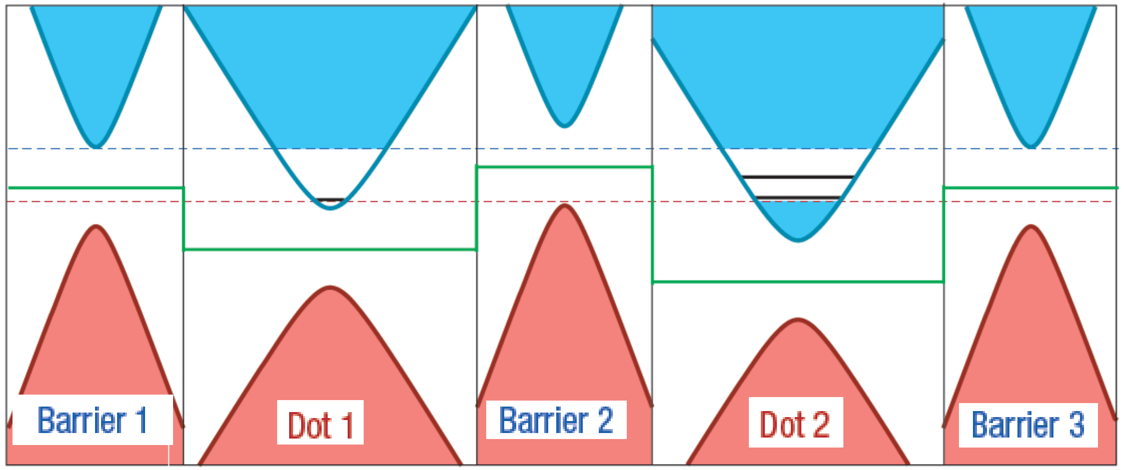
- **Predicted design: electrostatically confined graphene nanoribbons with armchair border**



DOUBLE-DOT

Exchange coupling between spins of electrons in Dot 1 and 2

$$H_{\text{exch}} = J\mathbf{S}_1 \cdot \mathbf{S}_2$$



with $J \sim$ t

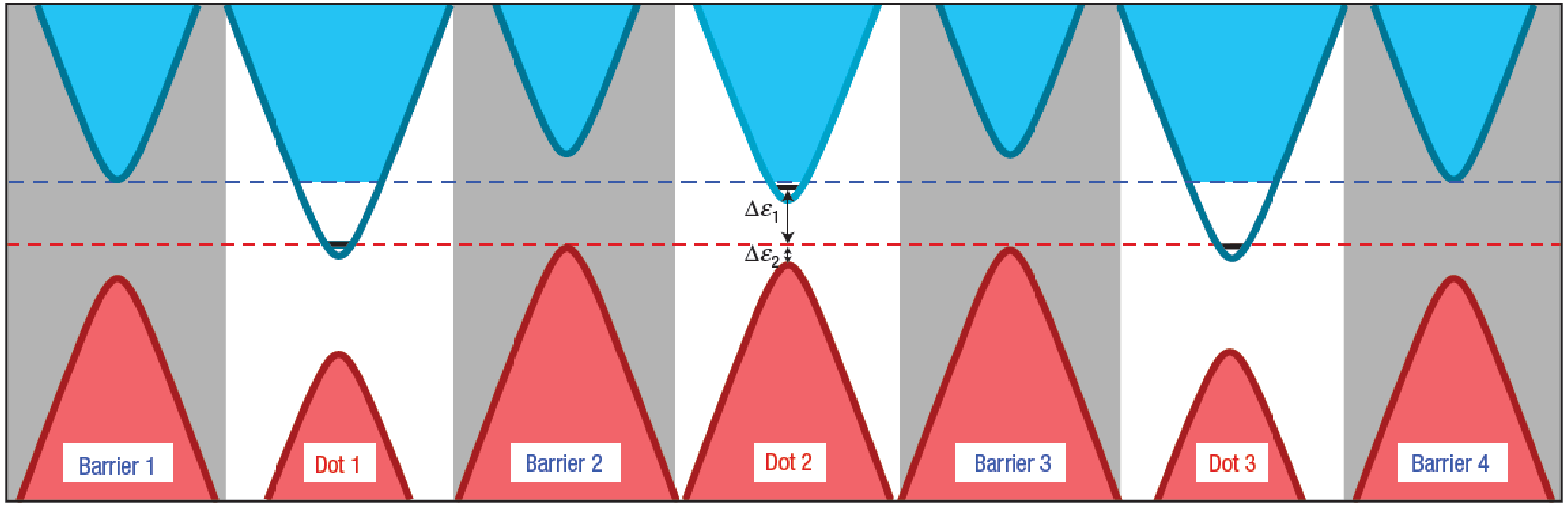
Tunneling between dots

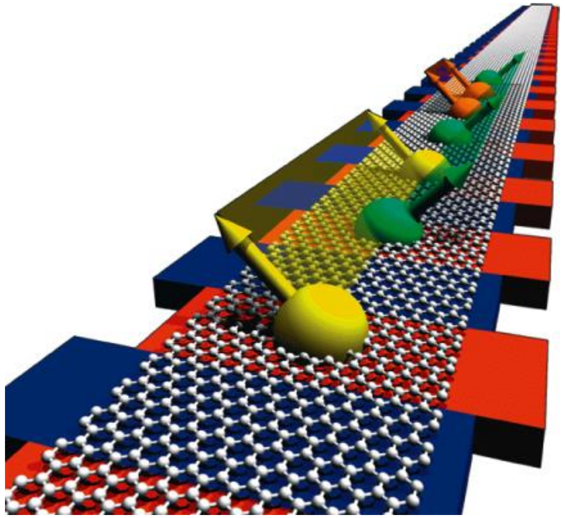
- Via cond. Band states (short distance, ~d)
- Via valence band (Klein T) long distance

Trauzettel et al. Nat. Physics, 2007

Spin Qubits in graphene

- **Long distance coupling of multiple graphene Qubits**





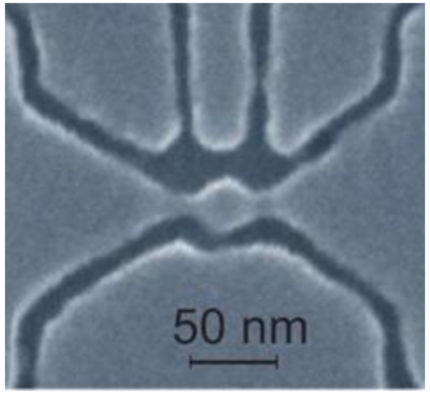
Strong coubling between Dot 1 and 3 via valence bands of barrier 2,3 and Dot 2 ($\Delta\varepsilon 2 \ll \Delta\varepsilon 1$)

Availability of long-range interactions is good for quantum error corrections

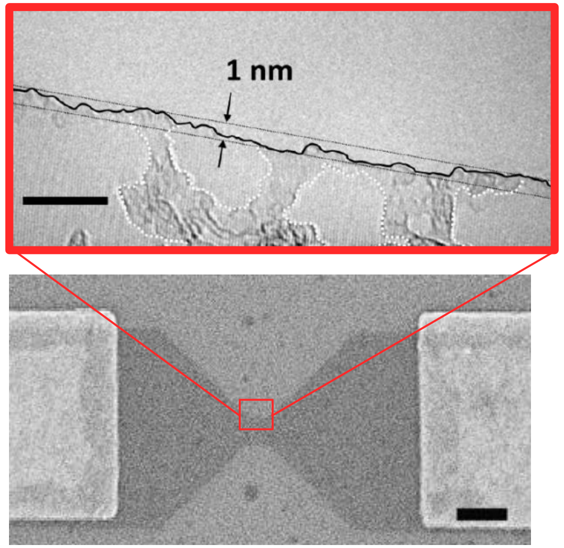
Trauzettel et al. Nat. Physics, 2007

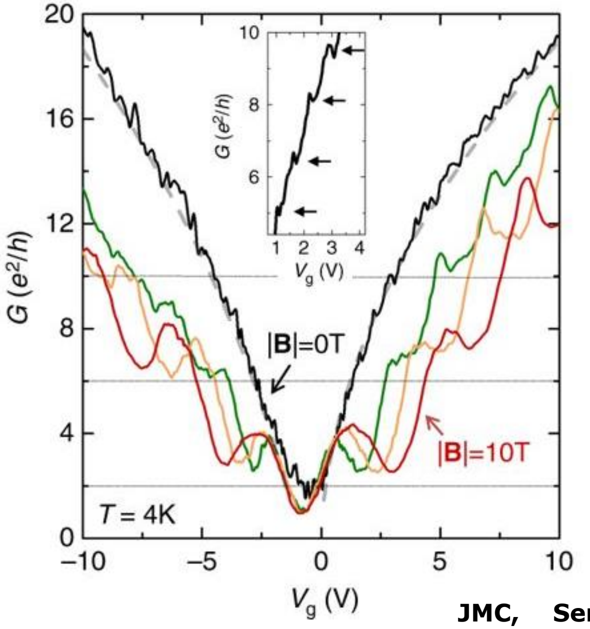
Spin Qubits in graphene: Experimental realization

Ponomarenko et al. Science 2008



- Top-down fabrication of graphene devices induces disorder in the material
- Disorder mainly occurs at edges (no controlled creation of ribbons with armchair edges)
- Disorder impedes the creation of spin quantum dots
- Even simpler graphene constrictions do not show clear quantization due to edge roughness

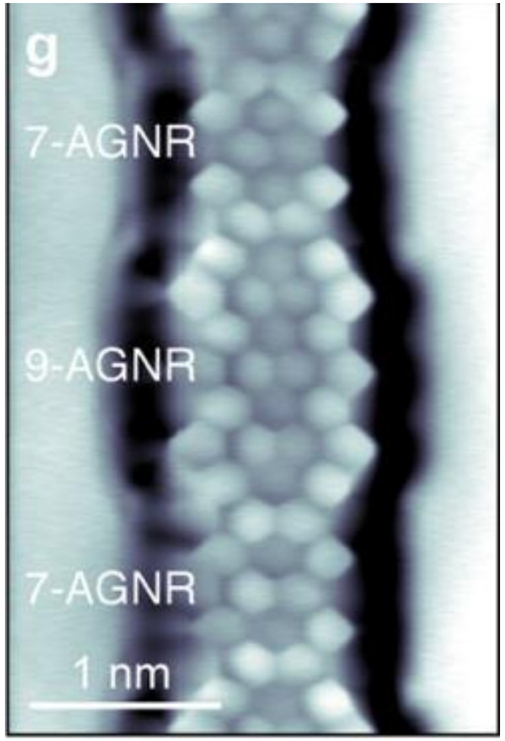


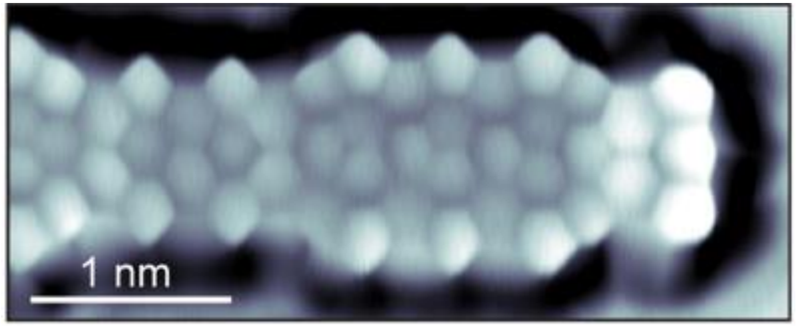


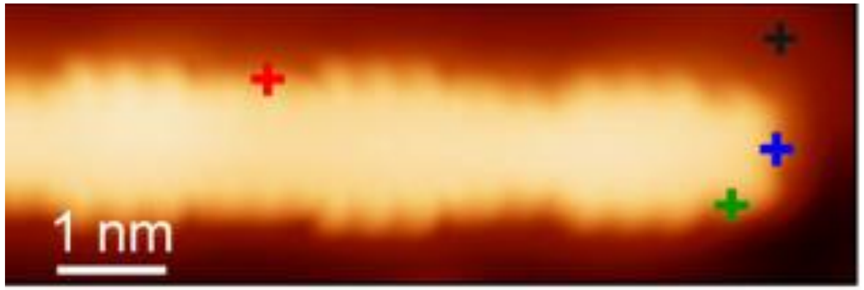
J.M. Caridad et al. Nat. Comm 2018

Spin Qubits in graphene: Experimental realization

Possible Solution: 1- Bottom up grow of gapped graphene nanostructures





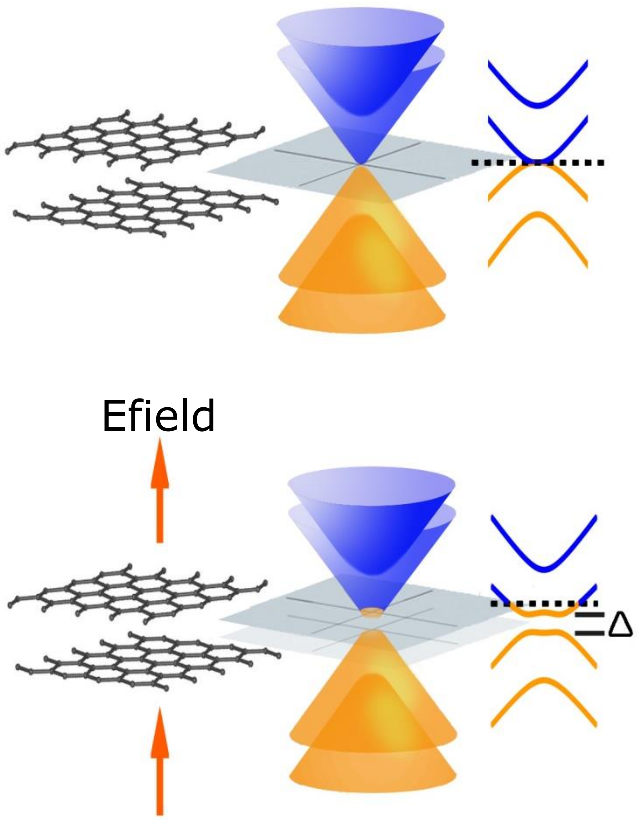


… but these samples are grown on a conducting substrate (metal)

Rizzo et al. Nature 2018

Spin Qubits in graphene: Experimental realization

Solution: 2- Electrostatic confinement in bilayer graphene

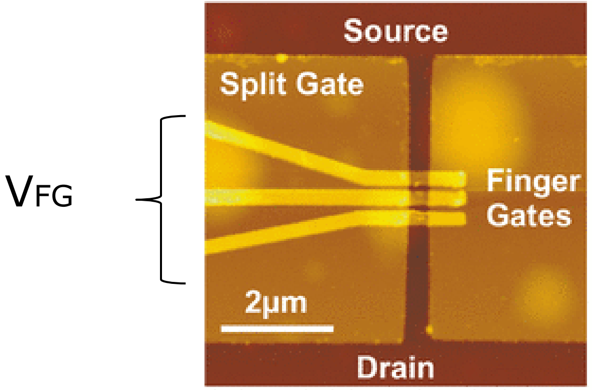


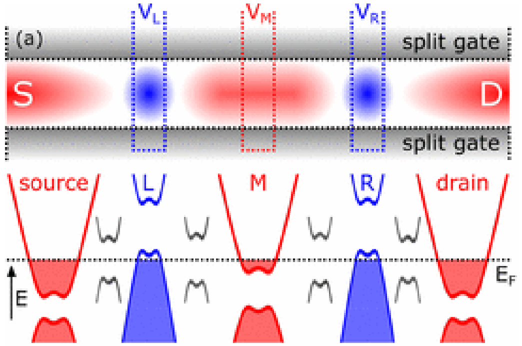
- Bilayer graphene is gapless (like graphene)
- Bilayer graphene develops a gap Δ in the presence of a perpendicular electric field

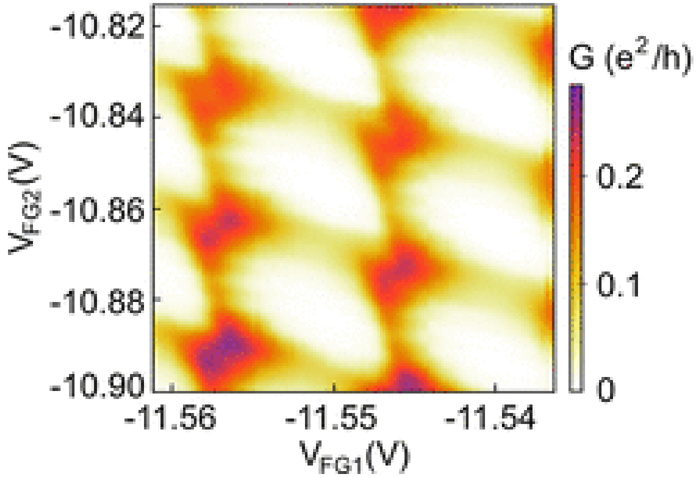
Zhang et al. Nature (2009)

Spin Qubits in graphene: Experimental realization

Coupled Qdots from bi-layer graphene recently demonstrated







** Next step: demonstrate spin Qubit operation*

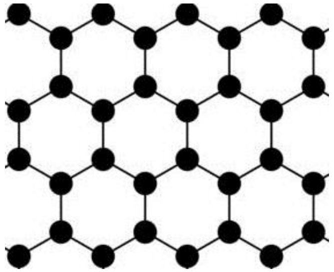
Banszerus et al. NanoLett (2018)

Eich et al. NanoLett (2018)

Outline: 2D Materials for Quantum Technologies

- Background: Qubits in conventional semiconductors

- Graphene* ⟶

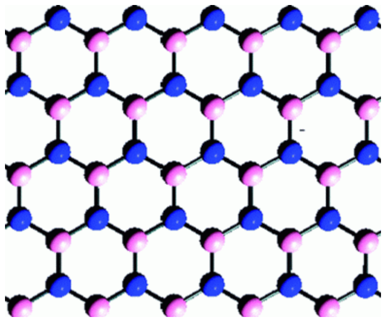


- C

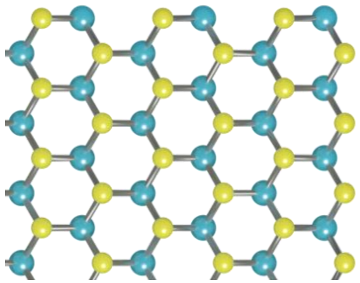
Devices:

- Spin Qubit *
- Valley Qubit
- Superconducting / Topol.protected
- Plasmons

- Other 2D materials (hBN, WSe2)



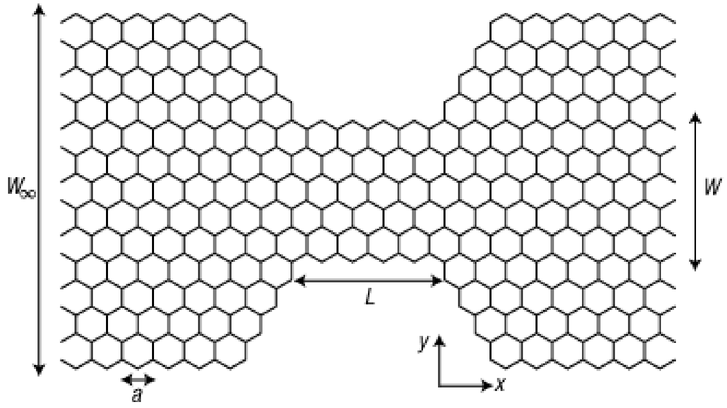
- N
- B

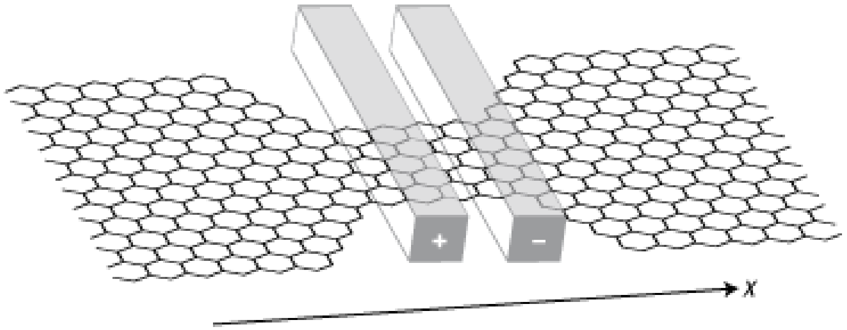


- W
- Se

Valley QuBits in graphene

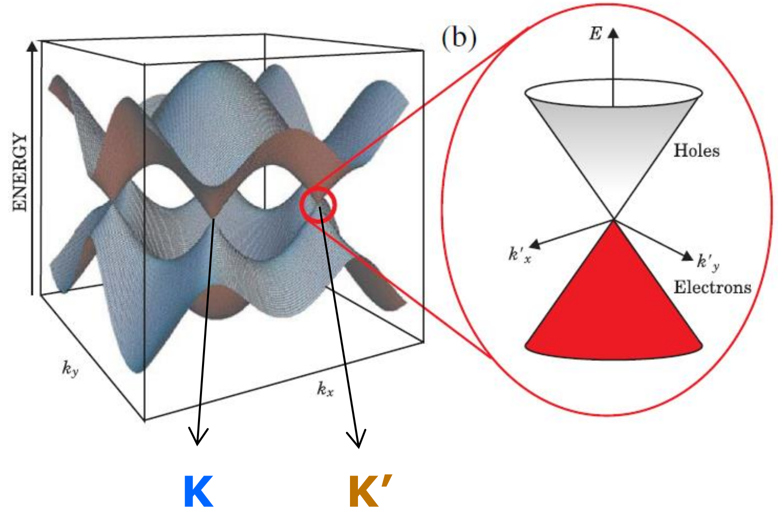
- **Predicted design: electrostatically confined graphene nanoribbons with zigzag border**





Rycerz et al. NatPhys (2007)

- Basis: **|K>** , **|K’>**
- Electron wavefunction: superposition **|K>** + $e^{i\theta}$ **|K’>**

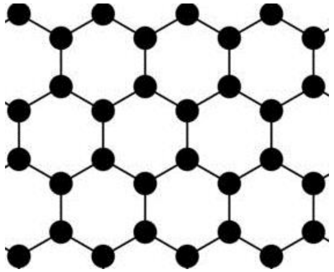


* Gates control the valley polarization of the electron

Outline: 2D Materials for Quantum Technologies

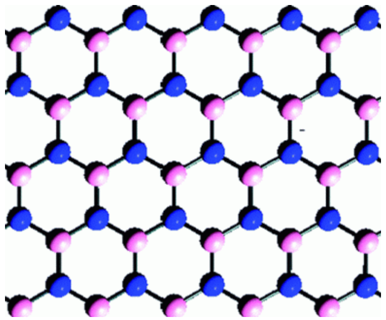
- Background: Qubits in conventional semiconductors

- Graphene* → Devices:
  - Spin Qubit *
  - Valley Qubit
  - Topologically protected
  - Plasmons

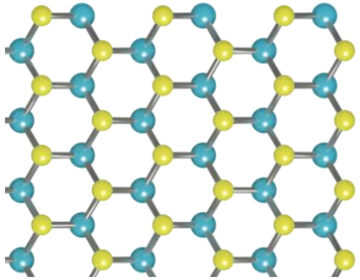


- C

- Other 2D materials (hBN, WSe2)



- N
- B



- W
- Se

Outline: 2D Materials for Quantum Technologies

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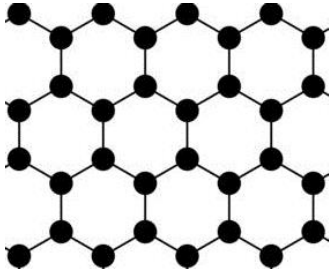

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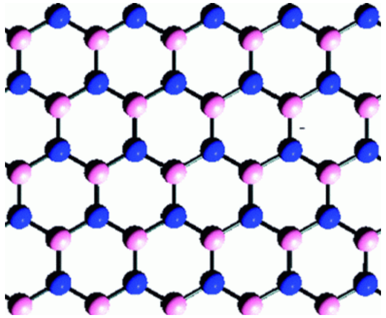
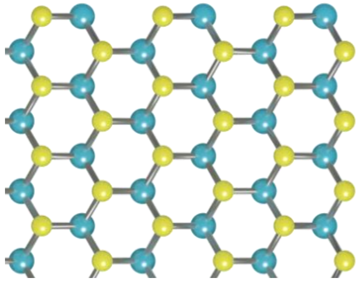


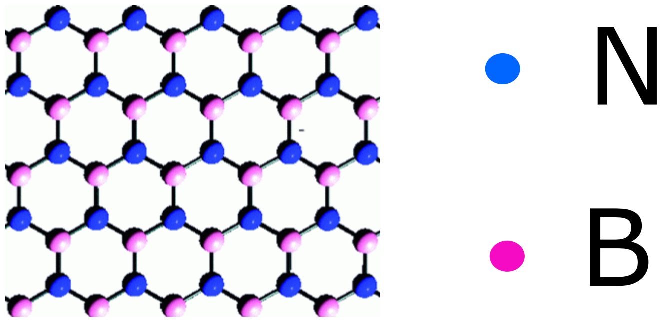
- N
- B

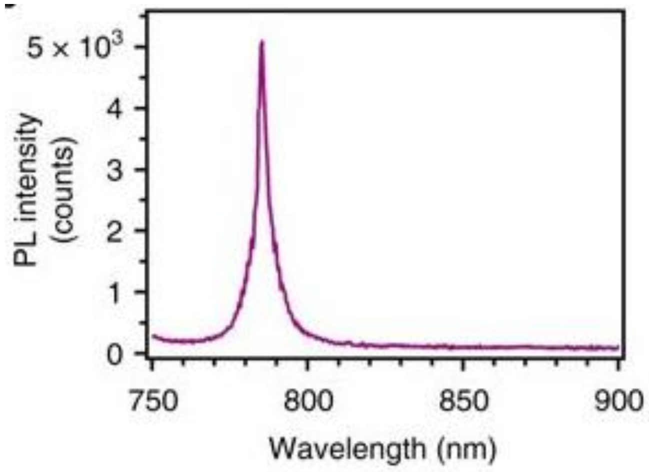


- W
- Se

Other 2D materials: hBN

- Quantum emitters in hexagonal boron nitride (hBN): atom-like properties but solid-state host environment!
- Similar to NV vacancies in diamond: spin-dependent photoluminescence
- High potential to engineer/locate QuBits (all surface material)

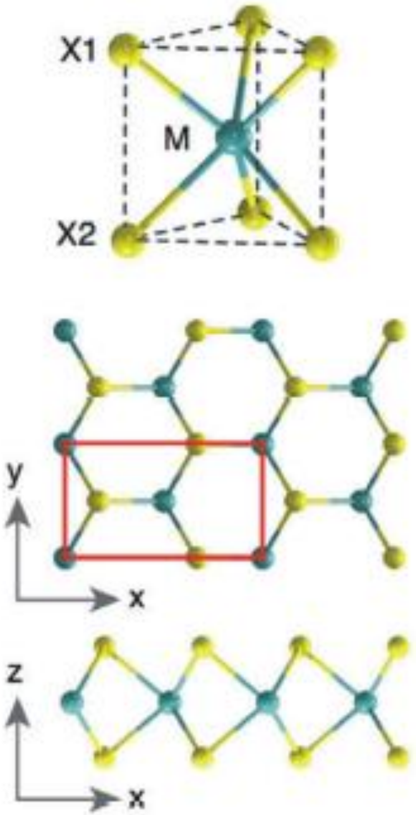




A. Exarhos, et al. Nat. Comm. (2019)

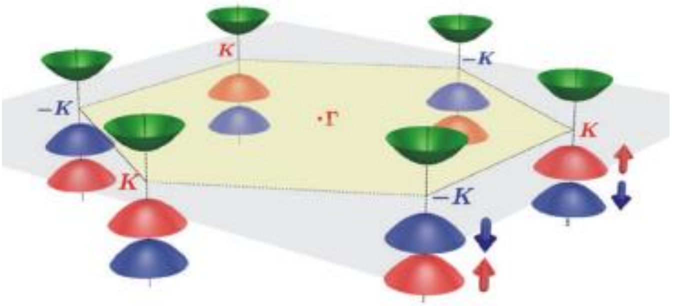
Other 2D materials: Transition metal Dichalcogenides (TMDC)

- Exploiting combination of internal degrees of fredom: Spin and valley



$$|\phi_c\rangle = |d_{z^2}\rangle$$
$$|\phi_v^\tau\rangle = \frac{1}{\sqrt{2}}(|d_{x^2-y^2}\rangle + i\tau\,|d_{xy}\rangle)$$

- Conduction and valence bands described by d-orbitals of metal (M)



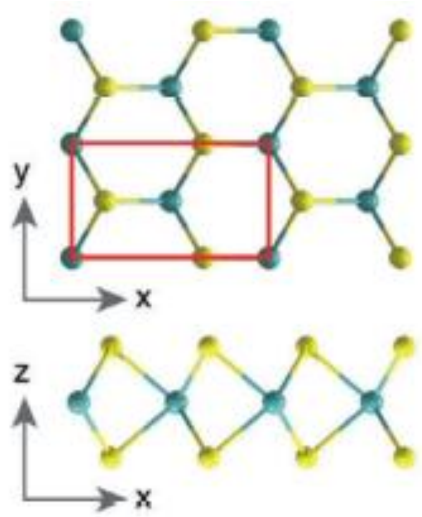
- Spin splitting in conduction and (mainly) valence band (↑ and ↓ spins can be accessed)

- Large spin orbit interaction lifts the valley degeneracy (**K** and **K'** valleys can be accessed)

Xiao, et al. PRL (2012)

Other 2D materials: Transition metal Dichalcogenides (TMDC)

- Easy manipulation of spin and valley degrees of freedom: magnetic means



- Equations of motion under the influence of external electric and magnetic fields

$$\dot{\mathbf{r}} = \frac{1}{\hbar}\frac{\partial E_n(\mathbf{k})}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \mathbf{\Omega_n}(\mathbf{k}) \longrightarrow$$

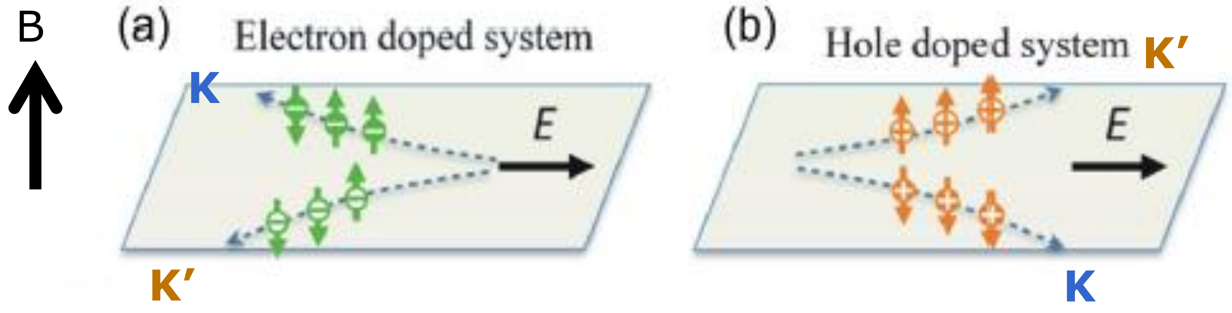
$$\hbar\dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}} \times \mathbf{B}$$

Dependent on valley index τ

1 (K) or -1 (K')

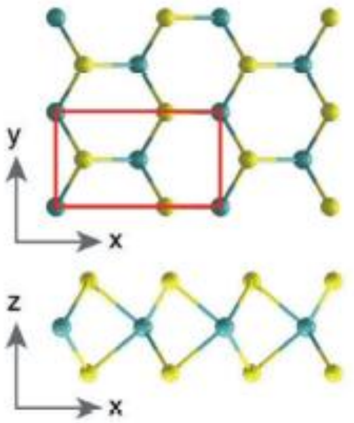
- Carriers in different valleys experience opposite transverse velocities -> Valley Hall effect

Xiao, et al. PRL (2012)



Other 2D materials: Transition metal Dichalcogenides (TMDC)

- Easy manipulation of spin and valley degrees of freedom: optical means



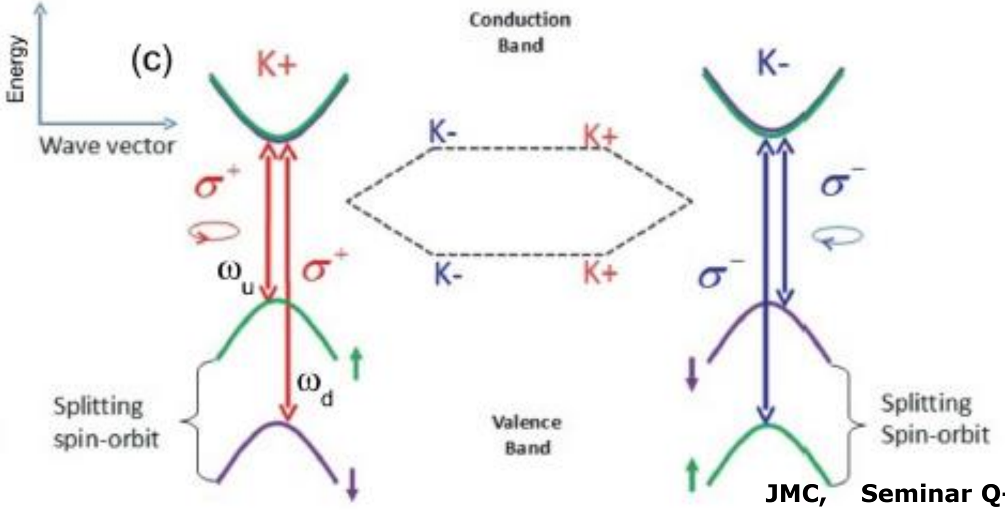
Xiao, et al. PRL (2012)

- Optical interband transitions with optical fields of circular polarization σ±: coupling strength

$$|P_{\pm}(\mathbf{k})|^2 = \frac{m_0^2 a^2 t^2}{\hbar^2}(1 \pm \tau)^2 \longrightarrow$$ Dependent on valley index τ : 1 (K) or -1 (K')

- Valley dependent selection rules:
  - σ+ → $|P_+(K')|^2=0$
  - σ- → $|P_-(K)|^2=0$

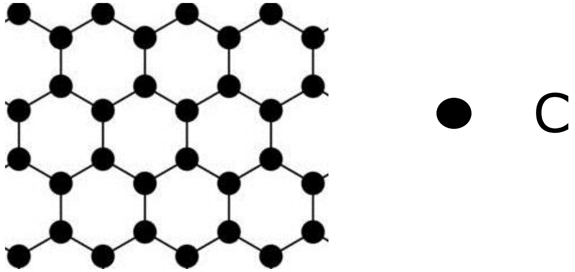
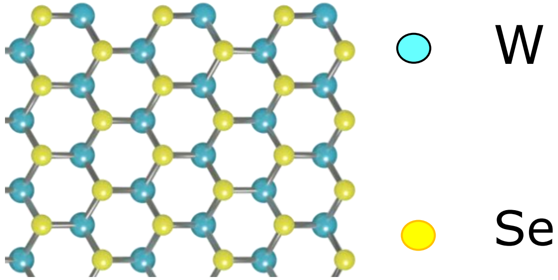
- Spin can be selectively excited



Graphene vs TMDCs materials for quantum technologies

Struck et al. PRB (2010)

Ye et al. NPJ Comp Mater. (2019)

	ADVANTAGES	*DISADVANTAGES*
	Decoherence time of ~100 ms (predicted)	Harder QuBit manipulation (specific devices to be built)
	Easier QuBit manipulation (specific devices to be built)	Decoherence time of ~10 ms (predicted)

Summary: 2D materials for quantum technologies

- **Several options to implement QuBits in 2D materials** (Spin, Valley Qbit, topologically-protected states, plasmons…)
- **Fast operation times** (faster than conventional semiconductors)
- **Longer decoherence times**
- **Long distance Qubit coupling** (graphene). Ideal for fault tolerant quantum computation
- **Easy QuBit manipulation** (TMDCs)

" Tomorrow's useful quantum computers won't be made with today's Qubits"

Charles Tahan, News & Views Nat. Nanotechnology, 101 (2019)

2D crystals are promising materials for tomorrow's quantum technologies

Thank you for your attention!