Two-dimensional materials

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Outline of the lectures

I. Graphene – band structure and topology

II. Symmetries of graphene and friends

III. Transition metal dichalcogenides (TMD)

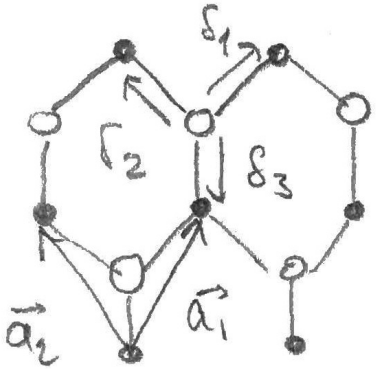
IV. Twisted bilayer graphene

Lecture 1

Graphene – band structure

Hexagonal (honeycomb) lattice

graphene = 2D plan of carbon atoms forming a honeycomb structure



○ A atoms
● B atoms

$$\vec{a}_1 = \frac{1}{2}\begin{pmatrix}\sqrt{3}\\3\end{pmatrix}$$

$$\vec{a}_2 = \frac{1}{2}\begin{pmatrix}-\sqrt{3}\\3\end{pmatrix}$$

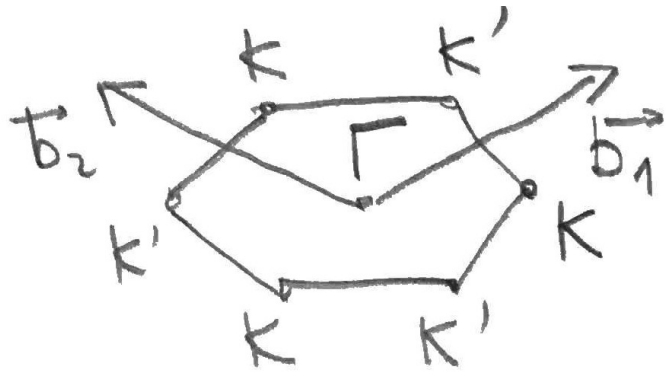
$$\vec{\delta}_3 = (0,-1)$$

$$\vec{\delta}_{1/2} = \left(\pm\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$$

$\vec{a}_1$ and $\vec{a}_2$ generate the whole lattice - with $\vec{\delta}_3$ connecting A and B atoms

Brillouin zone

BZ :



$$\vec{b}_1 = \frac{4\pi}{3}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$$

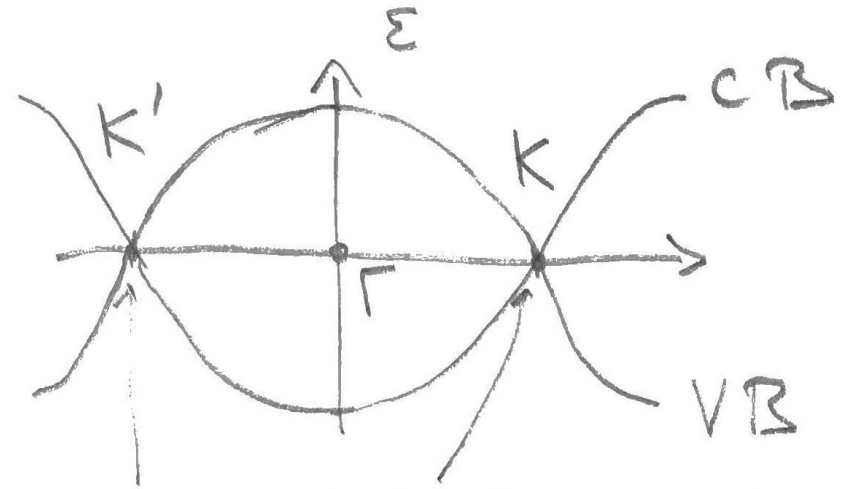
$$\vec{b}_2 = \frac{4\pi}{3}\left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$$

reciproqual vectors $\vec{b}_j \cdot \vec{a}_\ell = 2\pi \delta_{j,\ell}$

Gapless point $f(\vec{k} = \vec{K}) = 0$ with $\vec{K} = \frac{\vec{b}_1 - \vec{b}_2}{3}$

$\left(\frac{4\pi}{3\sqrt{3}}, 0\right)$

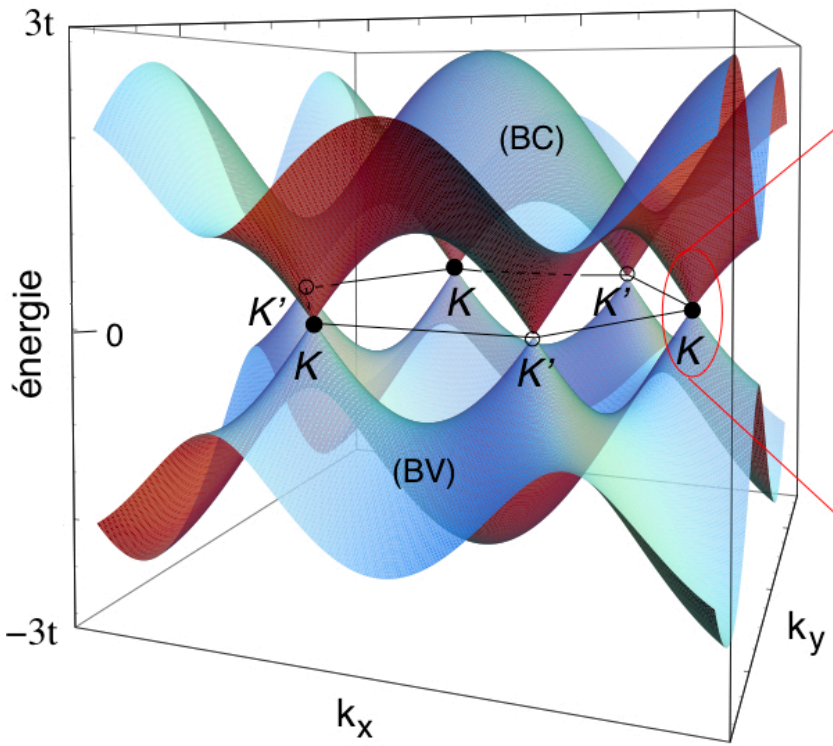
also $K' = K\, e^{i\pi/3}$, etc $f(K') = 0$

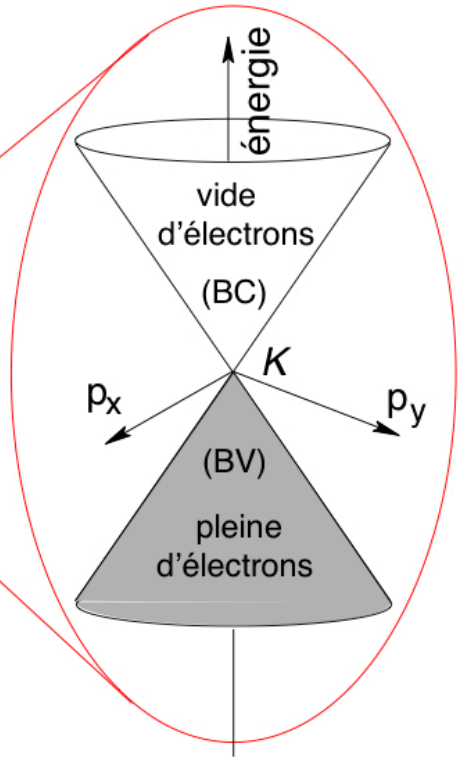


semi-metal (gapless) :

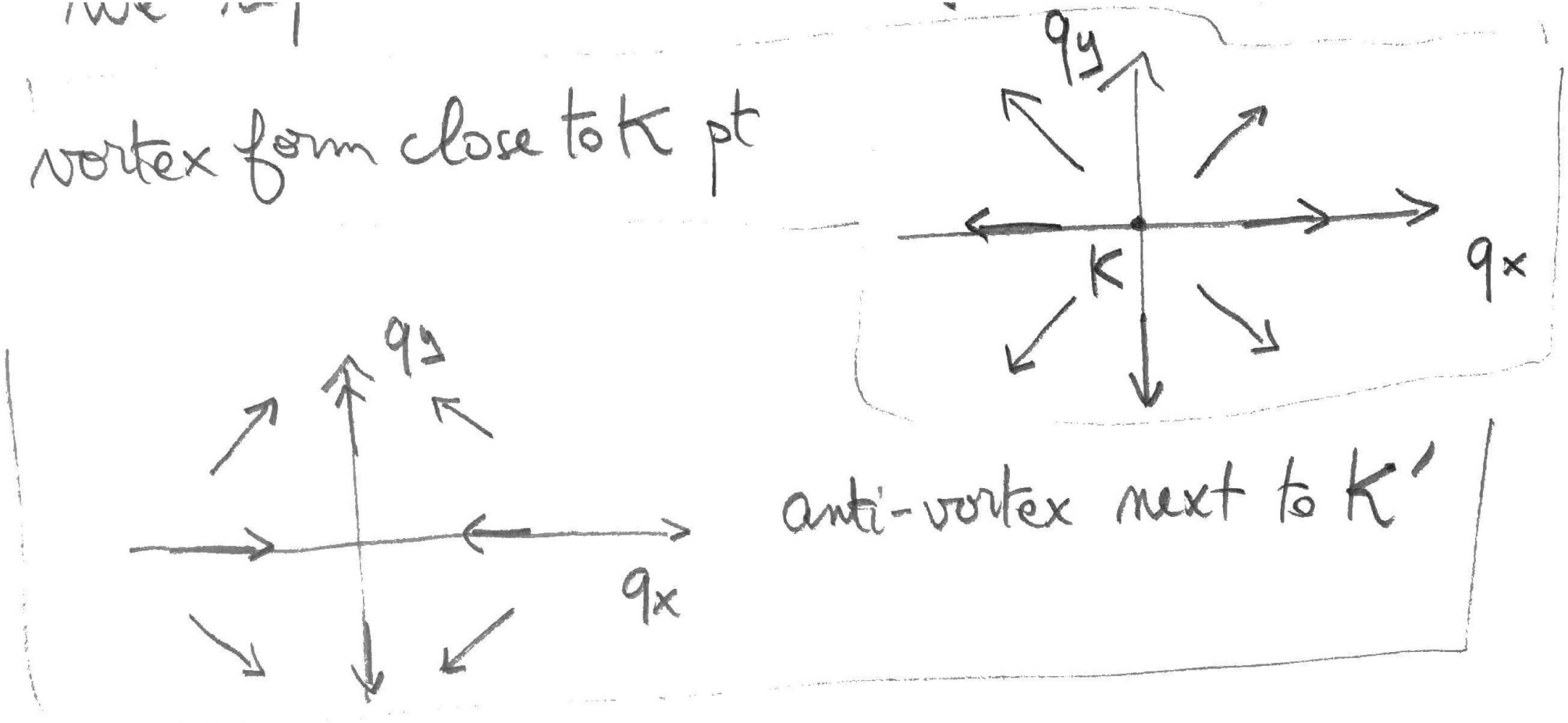
$\varepsilon_F = 0$

(1 é per unitcell per spin direction)





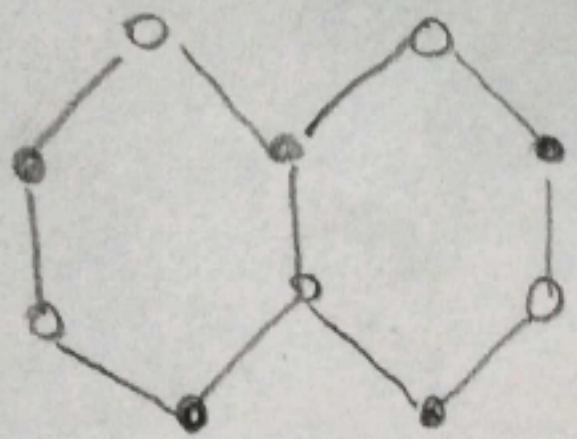
Vortex pattern close to K (K') point



Lecture 2

Symmetries of graphene

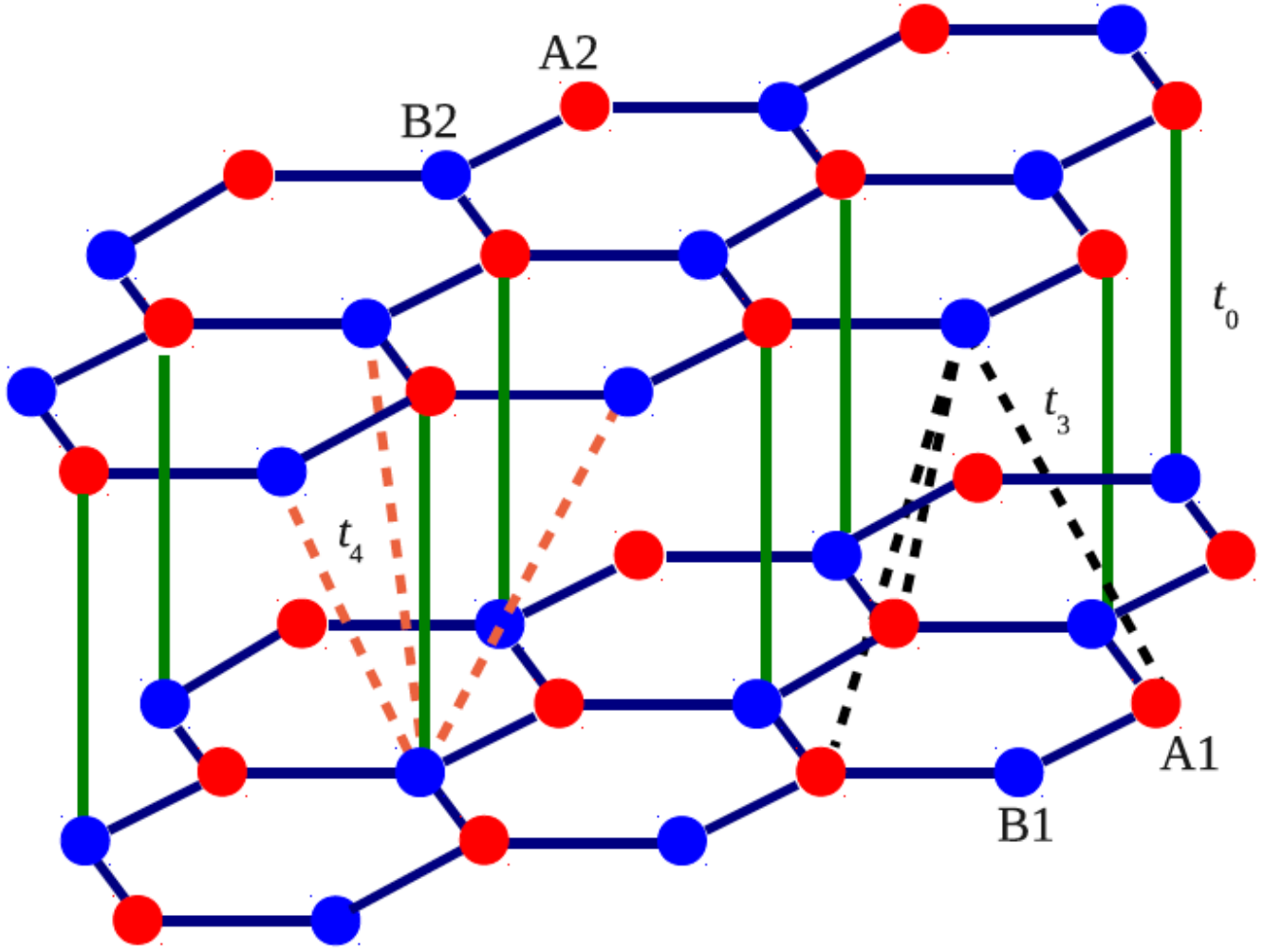
BN is very similar to graphene:
hexagonal 2D plane structure. Lattice constant within 1.5% to the one of graphene



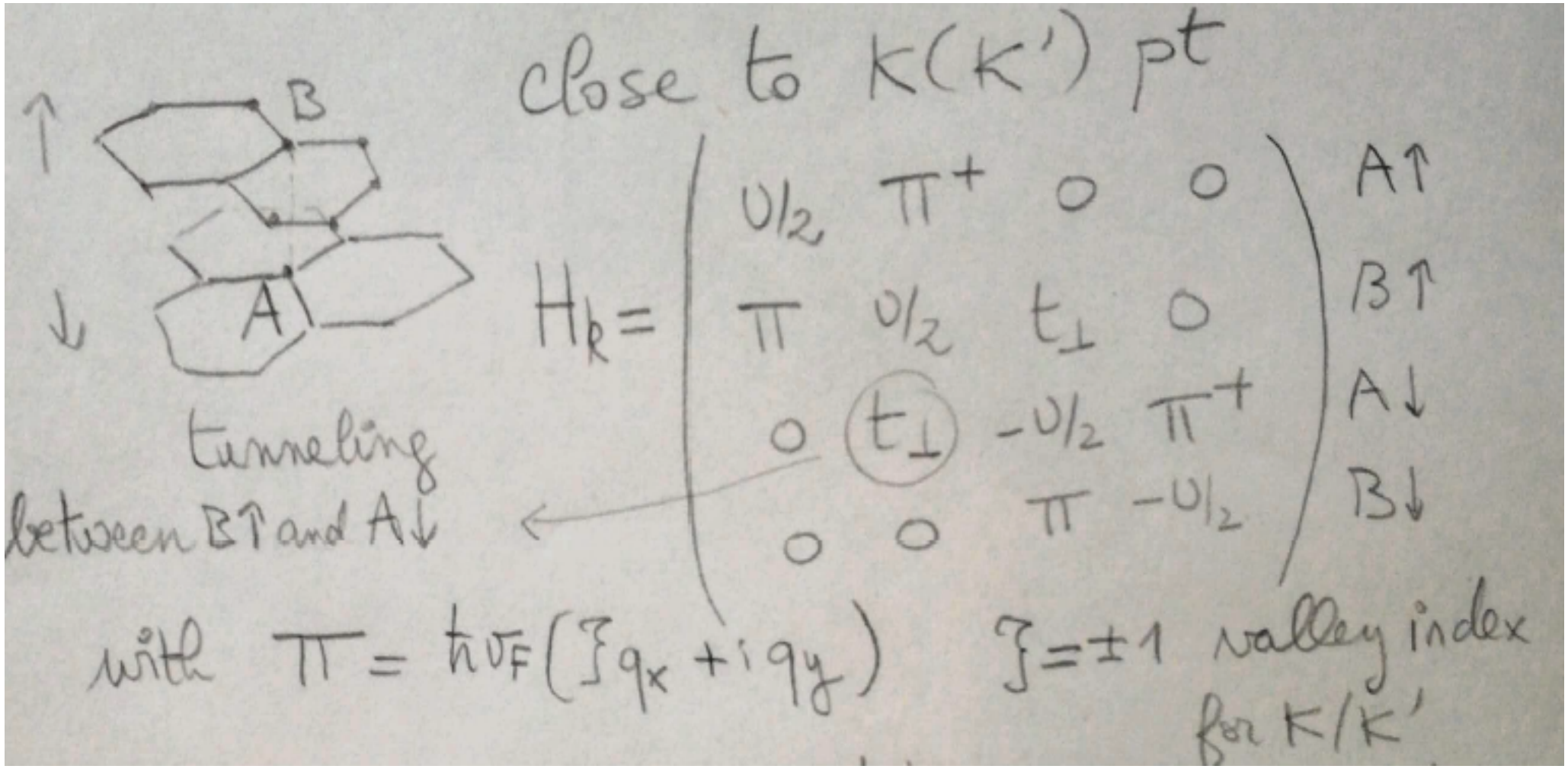
○ B
● N

but A and B sites are different

Bilayer graphene in Bernal stacking



Bilayer graphene in Bernal stacking



Group theory

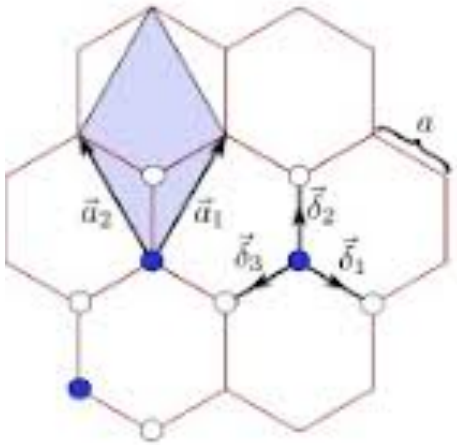
Space group

Symmetries of a crystalline lattice. Combination of lattice translations - forming a Bravais lattice - with point group operation such as reflection, rotation, improper rotation + screw axis and glide plane symmetries

(crystallographic) point group

Group of symmetry operations (rotations, plane symmetry, etc) which leave a point invariant

Examples of space groups



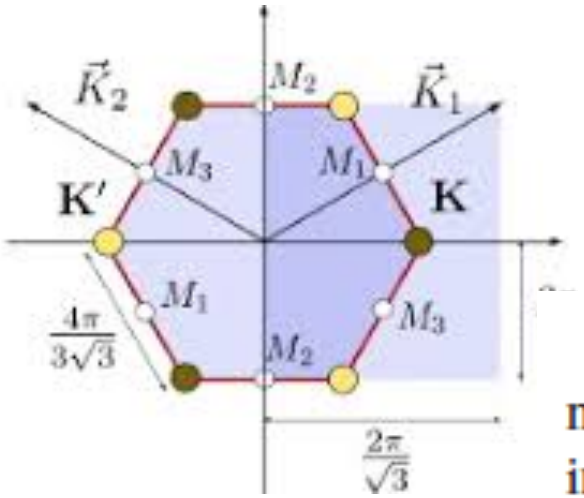
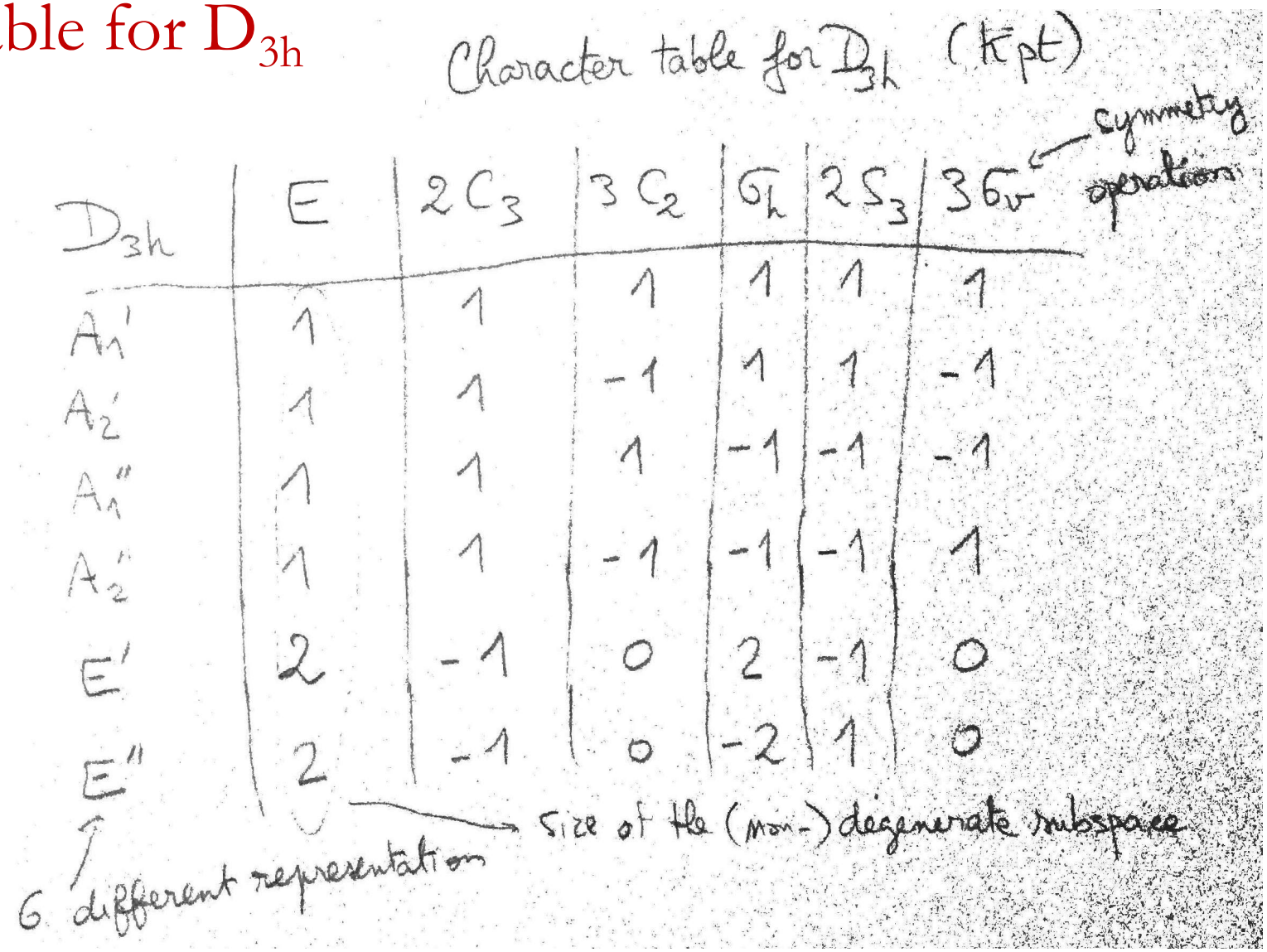


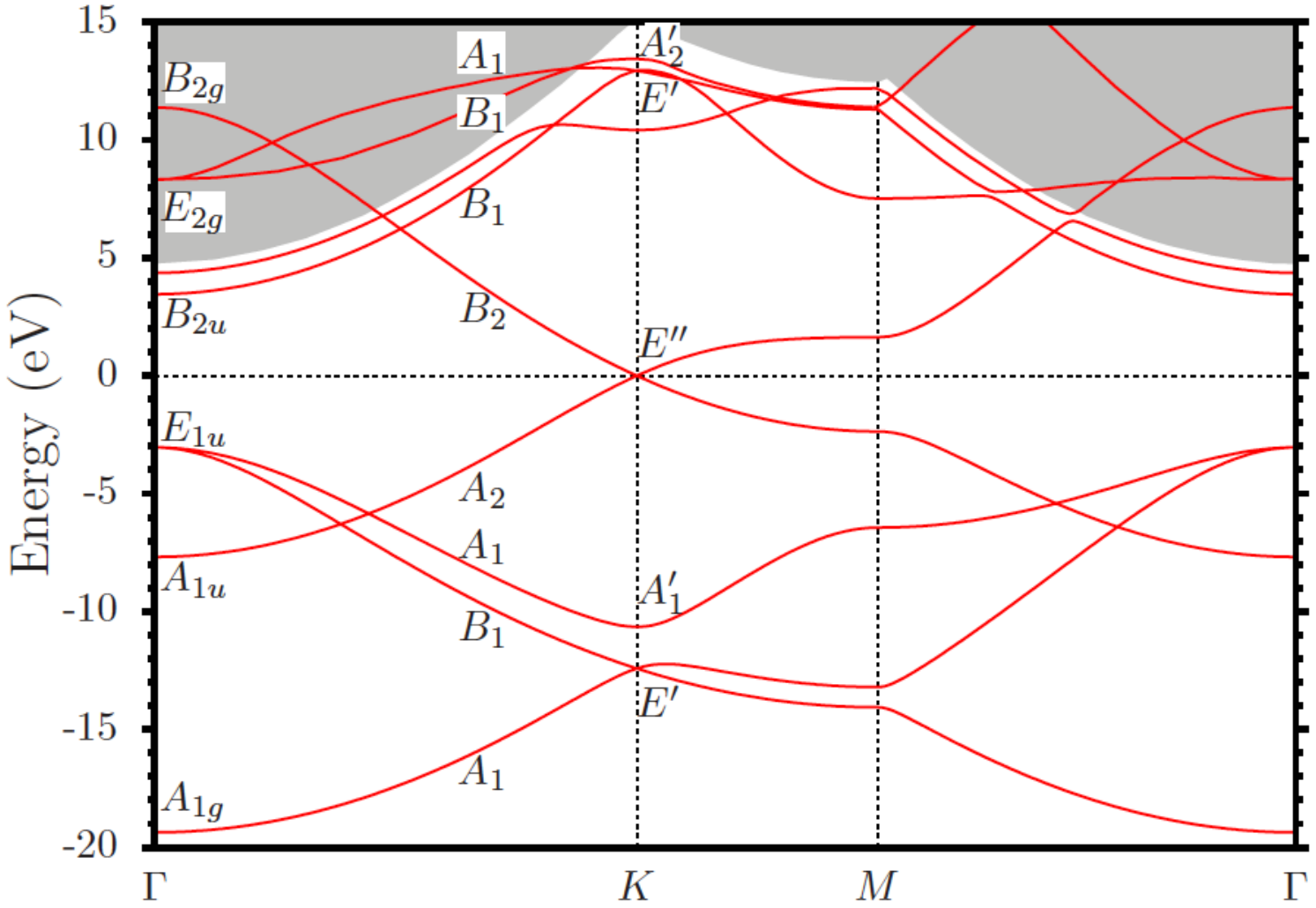
TABLE I. The space groups and wave-vector point groups for monolayer, N-layer graphene, and graphite (N infinite) at all points in the BZ.

	Space group	Γ	K (K')	M	T (T')	Σ	u
Monolayer	$P6/mmm$	D_{6h}	D_{3h}	D_{2h}	C_{2v}	C_{2v}	C_{1h}
N even	$P\bar{3}m1$	D_{3d}	D_3	C_{2h}	C_2	C_{1v}	C_1
N odd	$P\bar{6}m2$	D_{3h}	C_{3h}	C_{2v}	C_{1h}	C_{2v}	C_{1h}
N infinite	$P6_3/mmc$	D_{6h}	D_{3h}	D_{2h}	C_{2v}	C_{2v}	C_{1h}

Character table for D_{3h}

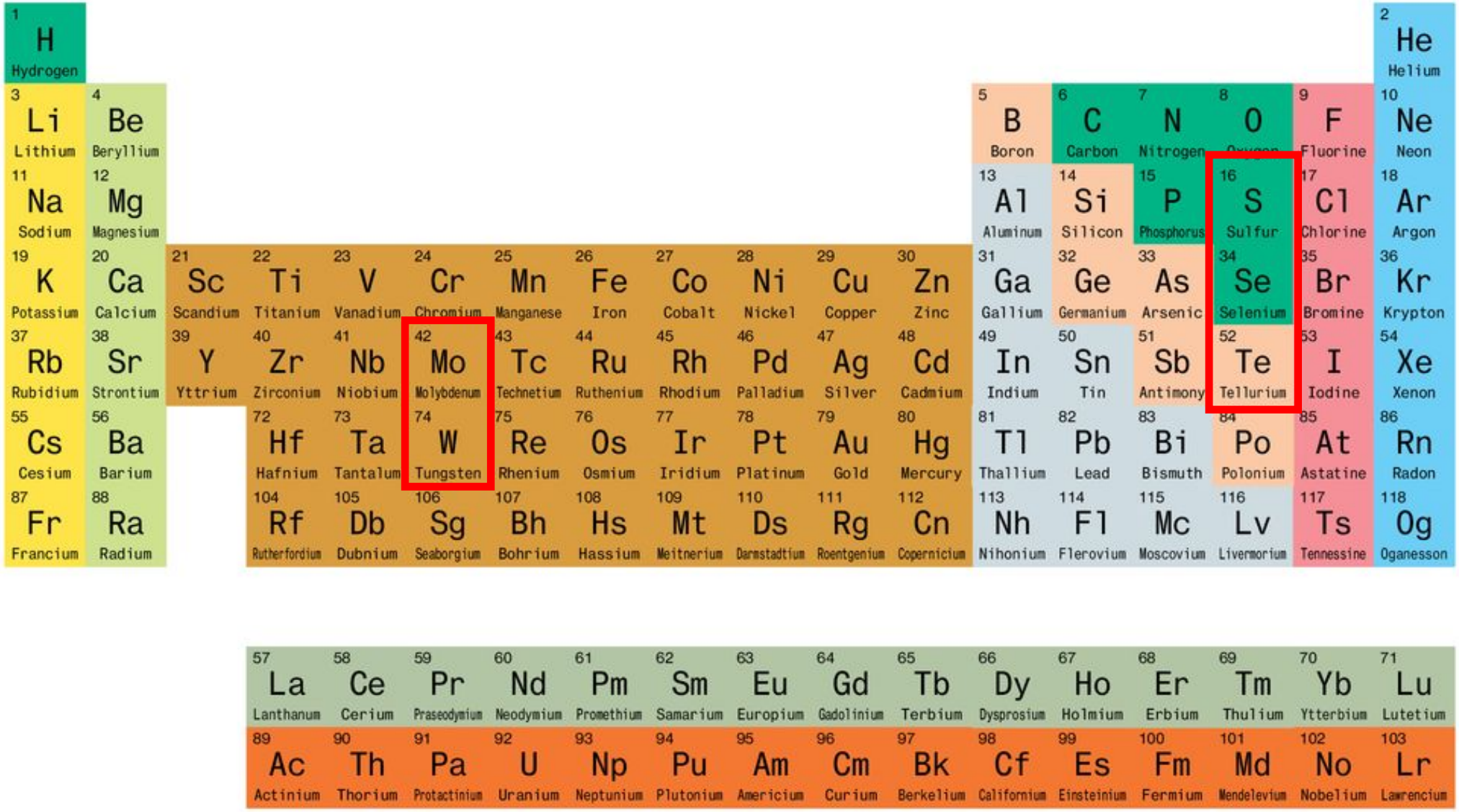


DFT calculation for monolayer graphene

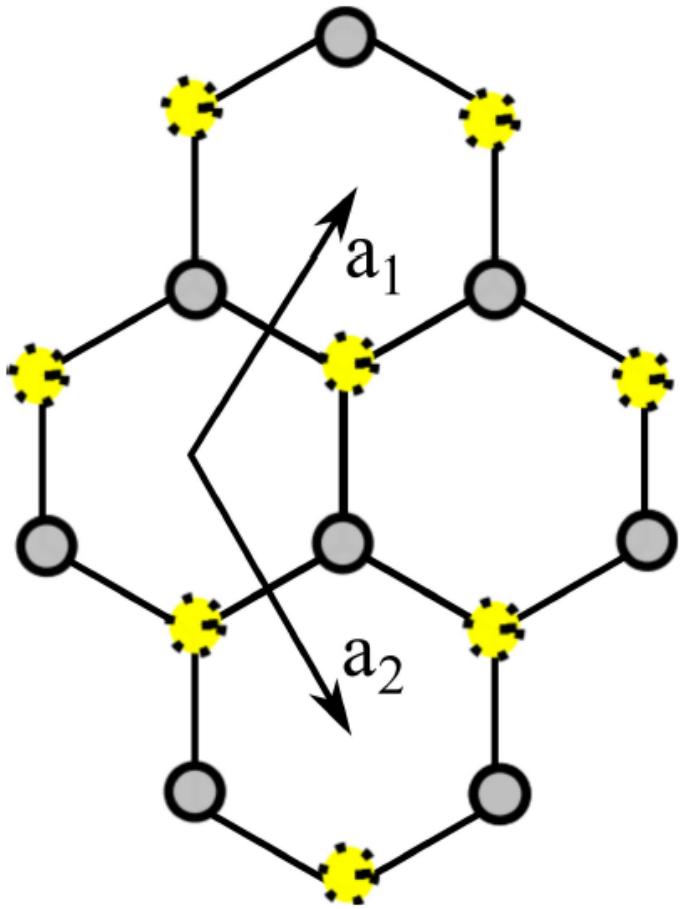


Lecture 3

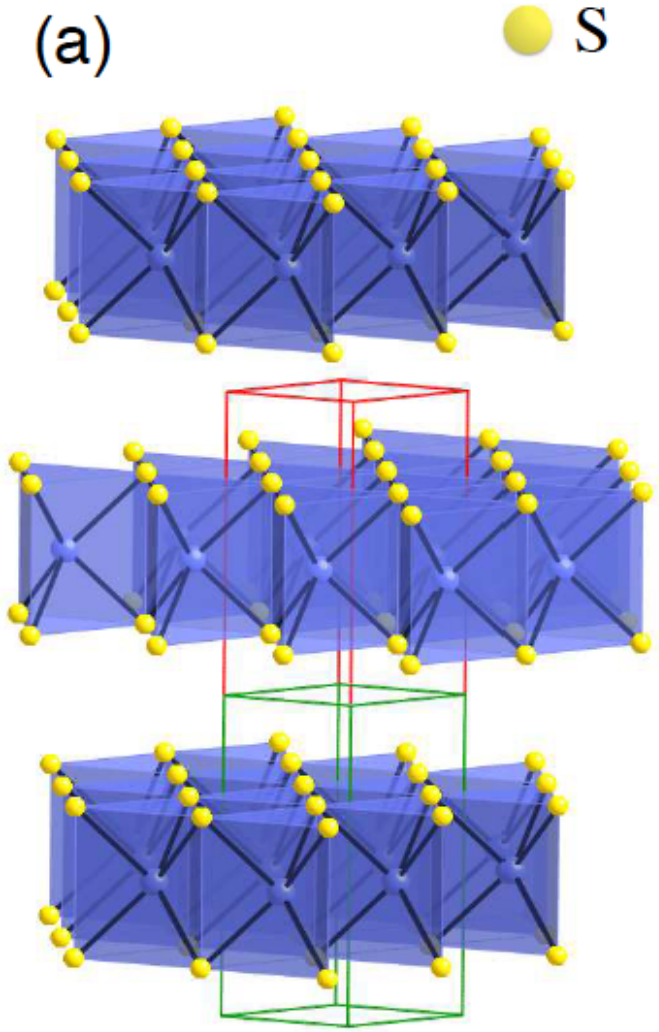
Transition metal dichalcogenides

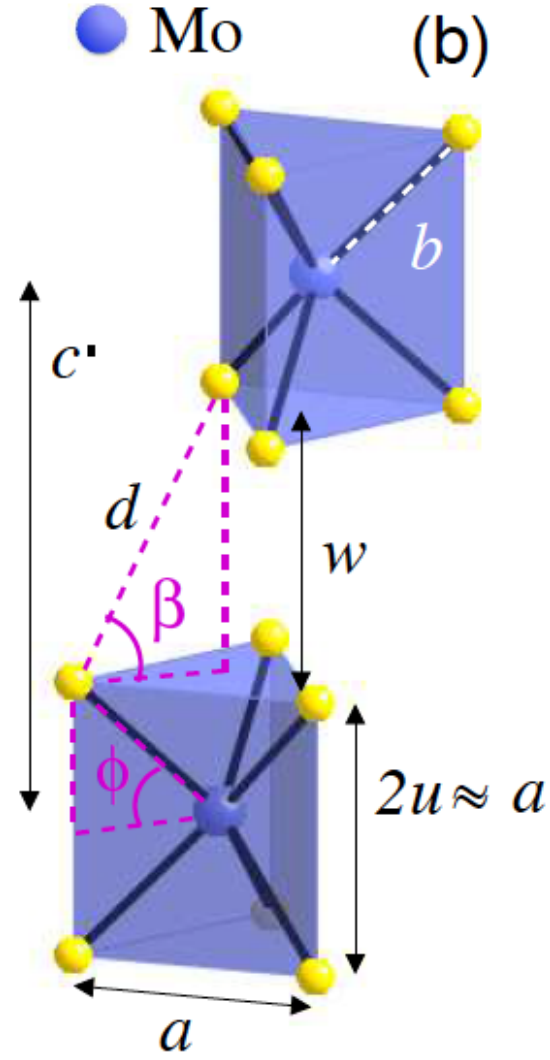

1 H Hydrogen
2 He Helium
3 Li Lithium
4 Be Beryllium
5 B Boron
6 C Carbon
7 N Nitrogen
8 O Oxygen
9 F Fluorine
10 Ne Neon
11 Na Sodium
12 Mg Magnesium
13 Al Aluminum
14 Si Silicon
15 P Phosphorus
16 S Sulfur
17 Cl Chlorine
18 Ar Argon
19 K Potassium
20 Ca Calcium
21 Sc Scandium
22 Ti Titanium
23 V Vanadium
24 Cr Chromium
25 Mn Manganese
26 Fe Iron
27 Co Cobalt
28 Ni Nickel
29 Cu Copper
30 Zn Zinc
31 Ga Gallium
32 Ge Germanium
33 As Arsenic
34 Se Selenium
35 Br Bromine
36 Kr Krypton
37 Rb Rubidium
38 Sr Strontium
39 Y Yttrium
40 Zr Zirconium
41 Nb Niobium
42 Mo Molybdenum
43 Tc Technetium
44 Ru Ruthenium
45 Rh Rhodium
46 Pd Palladium
47 Ag Silver
48 Cd Cadmium
49 In Indium
50 Sn Tin
51 Sb Antimony
52 Te Tellurium
53 I Iodine
54 Xe Xenon
55 Cs Cesium
56 Ba Barium
72 Hf Hafnium
73 Ta Tantalum
74 W Tungsten
75 Re Rhenium
76 Os Osmium
77 Ir Iridium
78 Pt Platinum
79 Au Gold
80 Hg Mercury
81 Tl Thallium
82 Pb Lead
83 Bi Bismuth
84 Po Polonium
85 At Astatine
86 Rn Radon
87 Fr Francium
88 Ra Radium
104 Rf Rutherfordium
105 Db Dubnium
106 Sg Seaborgium
107 Bh Bohrium
108 Hs Hassium
109 Mt Meitnerium
110 Ds Darmstadtium
111 Rg Roentgenium
112 Cn Copernicium
113 Nh Nihonium
114 Fl Flerovium
115 Mc Moscovium
116 Lv Livermorium
117 Ts Tennessine
118 Og Oganesson
57 La Lanthanum
58 Ce Cerium
59 Pr Praseodymium
60 Nd Neodymium
61 Pm Promethium
62 Sm Samarium
63 Eu Europium
64 Gd Gadolinium
65 Tb Terbium
66 Dy Dysprosium
67 Ho Holmium
68 Er Erbium
69 Tm Thulium
70 Yb Ytterbium
71 Lu Lutetium
89 Ac Actinium
90 Th Thorium
91 Pa Protactinium
92 U Uranium
93 Np Neptunium
94 Pu Plutonium
95 Am Americium
96 Cm Curium
97 Bk Berkelium
98 Cf Californium
99 Es Einsteinium
100 Fm Fermium
101 Md Mendelevium
102 No Nobelium
103 Lr Lawrencium

MoS_2

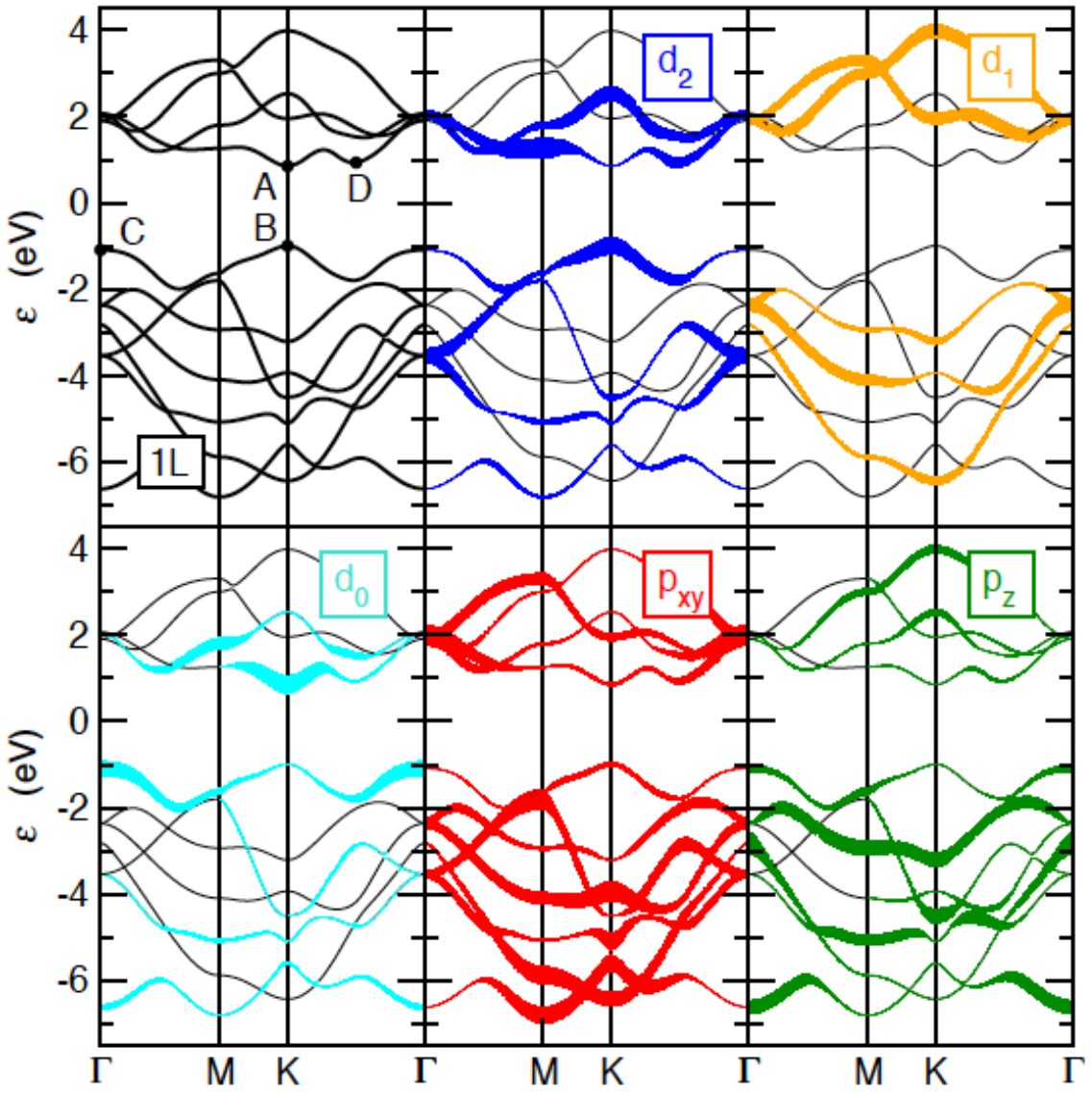


Top view





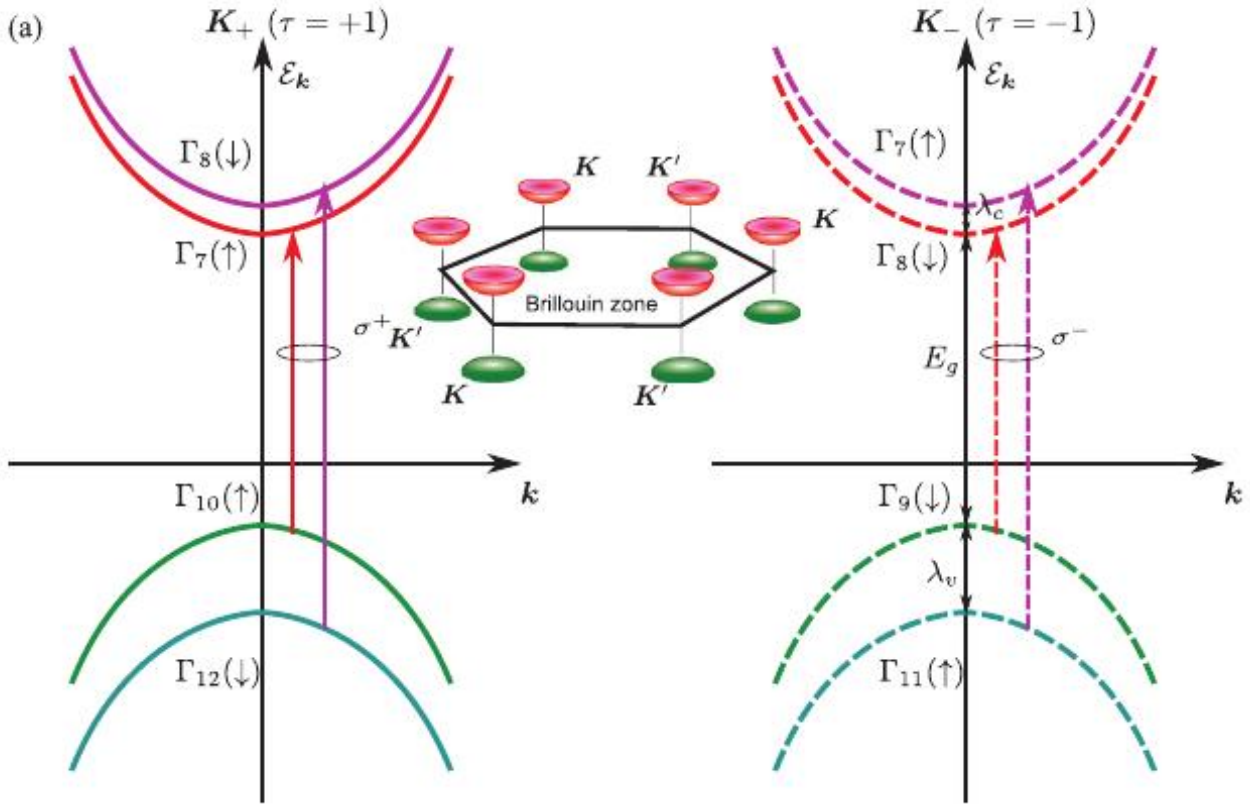
DFT for MoS_2

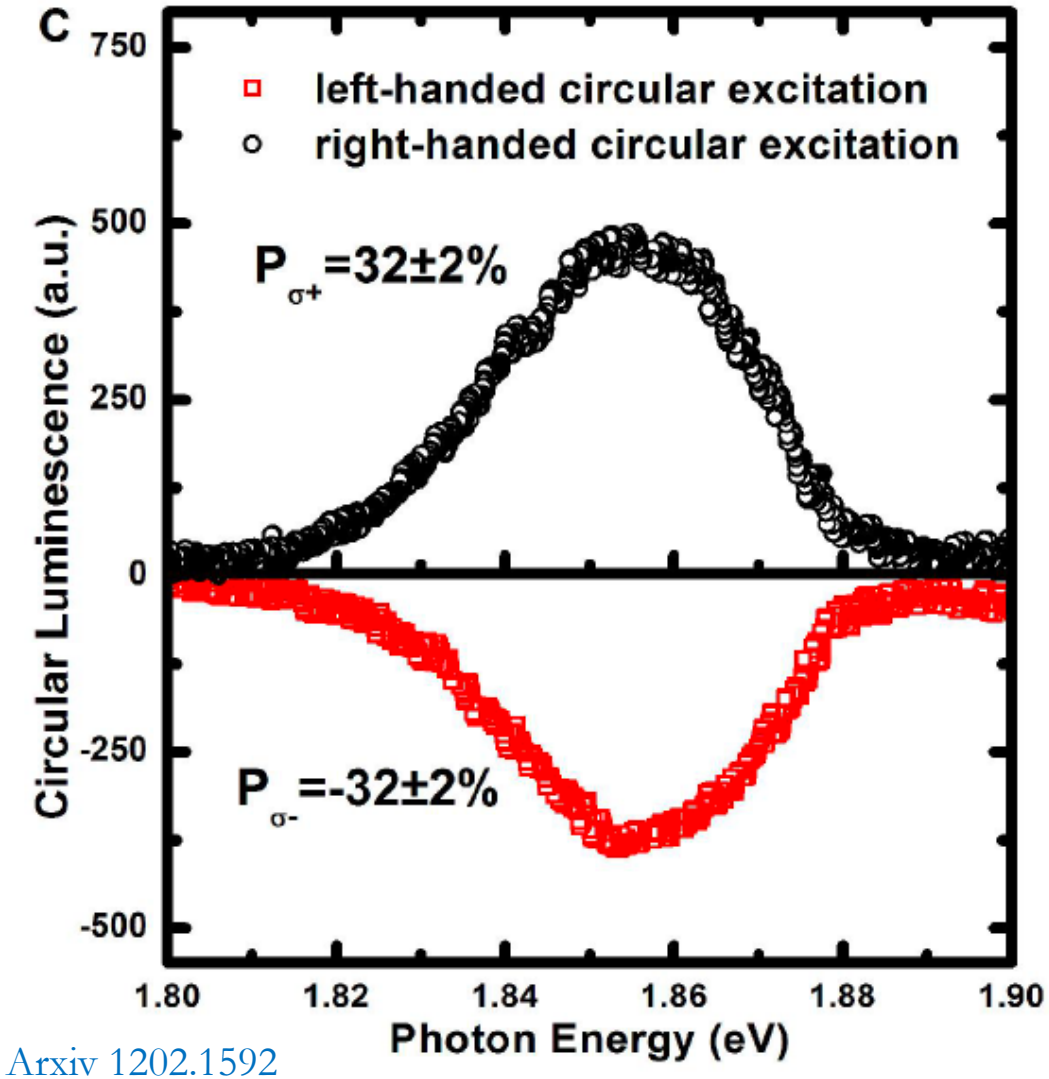


Character table for C_{3h}

$\overline{6}\,(C_{3h})$	E	C_3	C_3^2	σ_h	S_3	$\sigma_h C_3^2$
A'	1	1	1	1	1	1
A''	1	1	1	-1	-1	-1
E_1'	1	ω	ω^2	1	ω	ω^2
E_2'	1	ω^2	ω	1	ω^2	ω
E_1''	1	ω	ω^2	-1	$-\omega$	$-\omega^2$
E_2''	1	ω^2	ω	-1	$-\omega^2$	$-\omega$

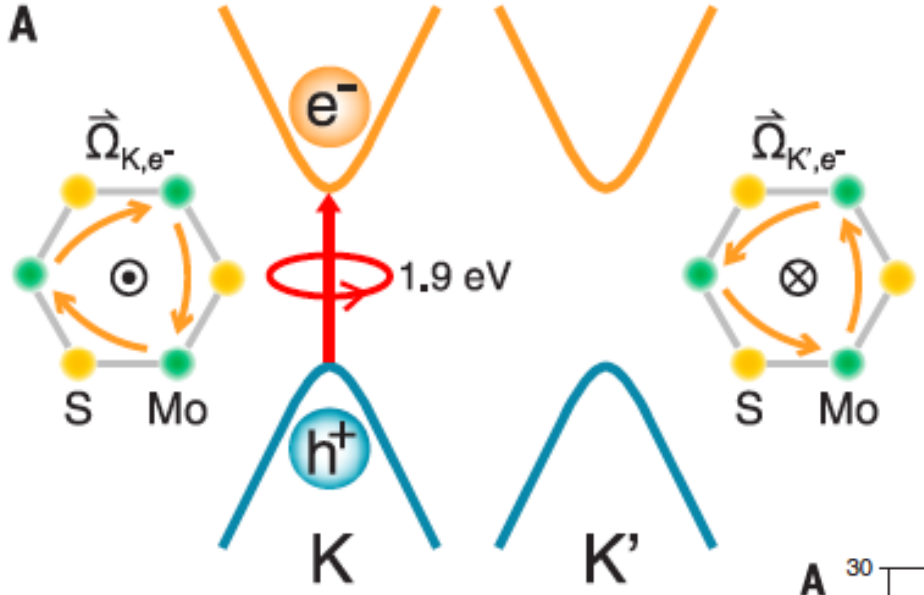
Circular dichroism

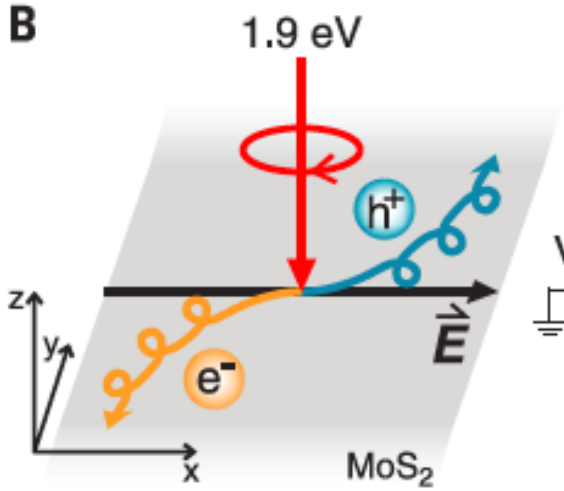


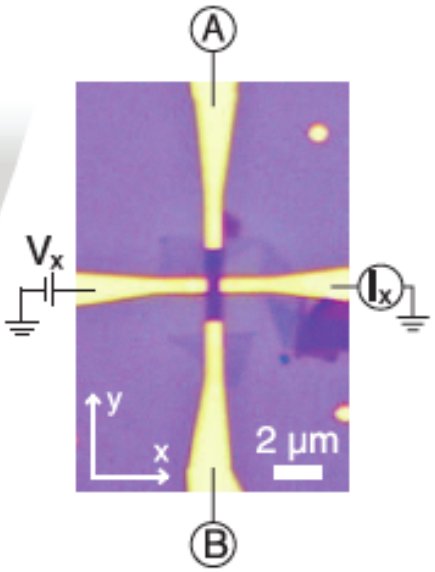


Zeng, Cui et al. Arxiv 1202.1592

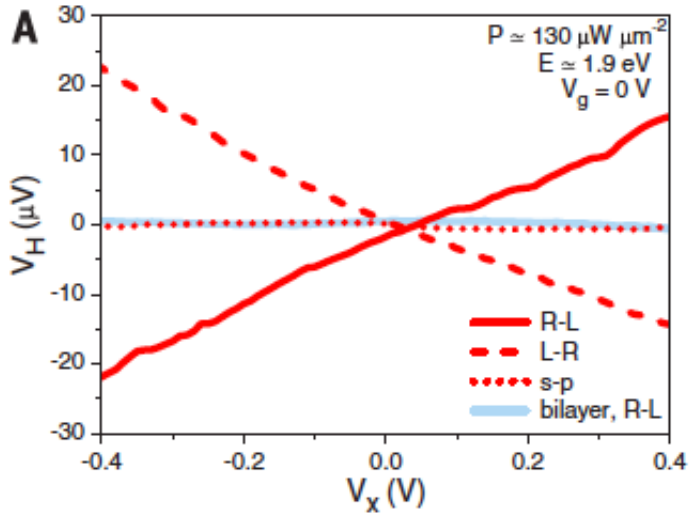
Valley Hall effect







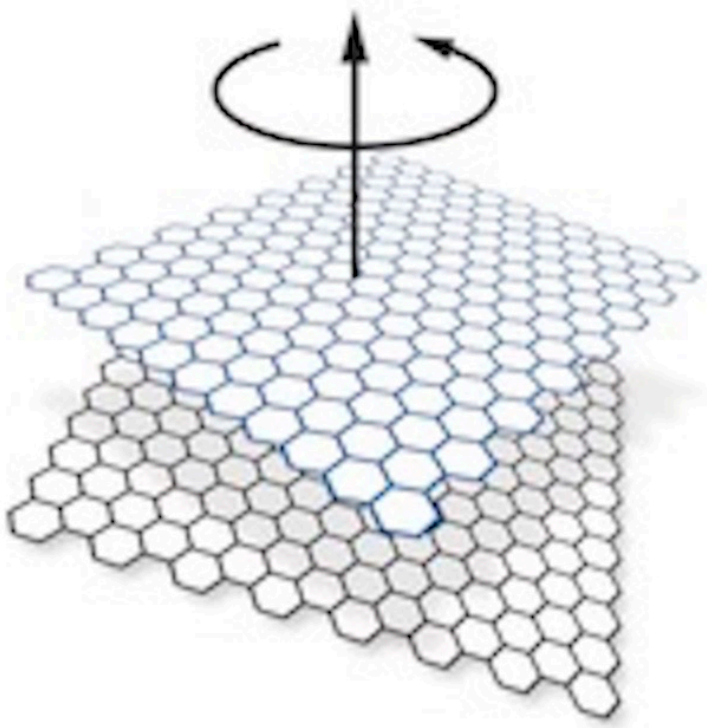
Mak, Mac Euen et al., Science (2014)



Lecture 4

Twisted bilayer graphene

Twisted bilayer graphene



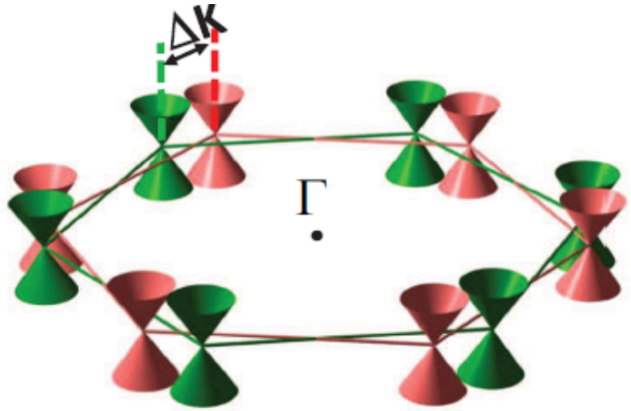
Simple and straightforward principle:

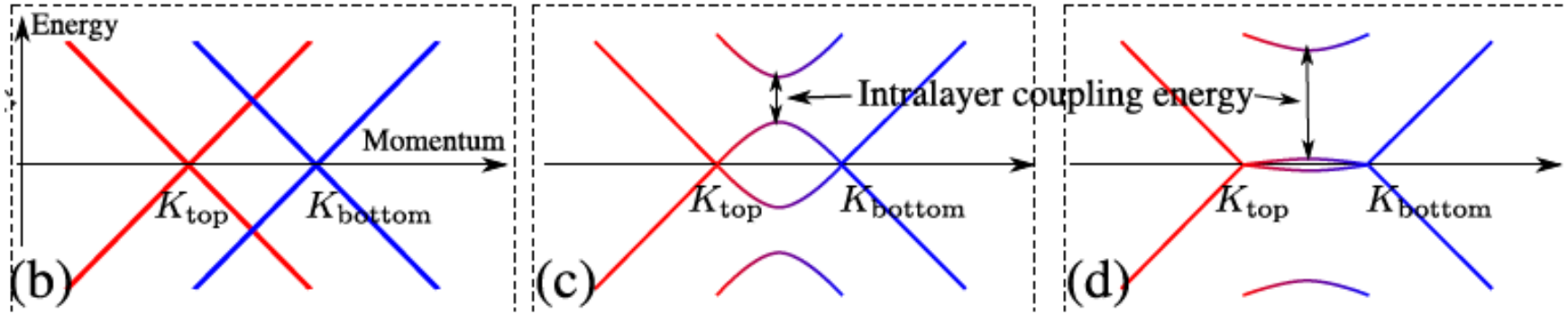
Overlaying two honeycomb lattices (graphene)

with a small relative twist

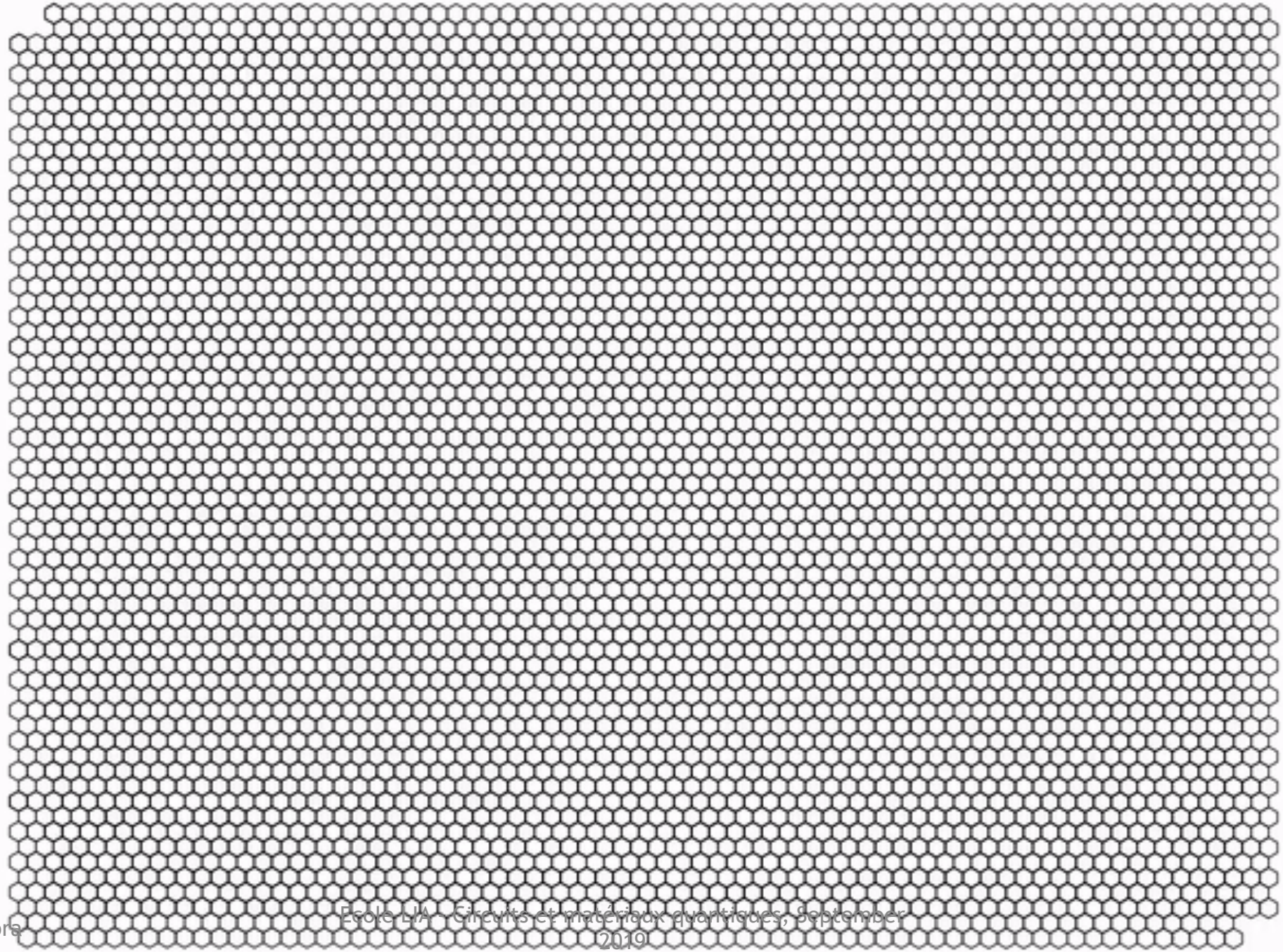
Creates a Moiré pattern

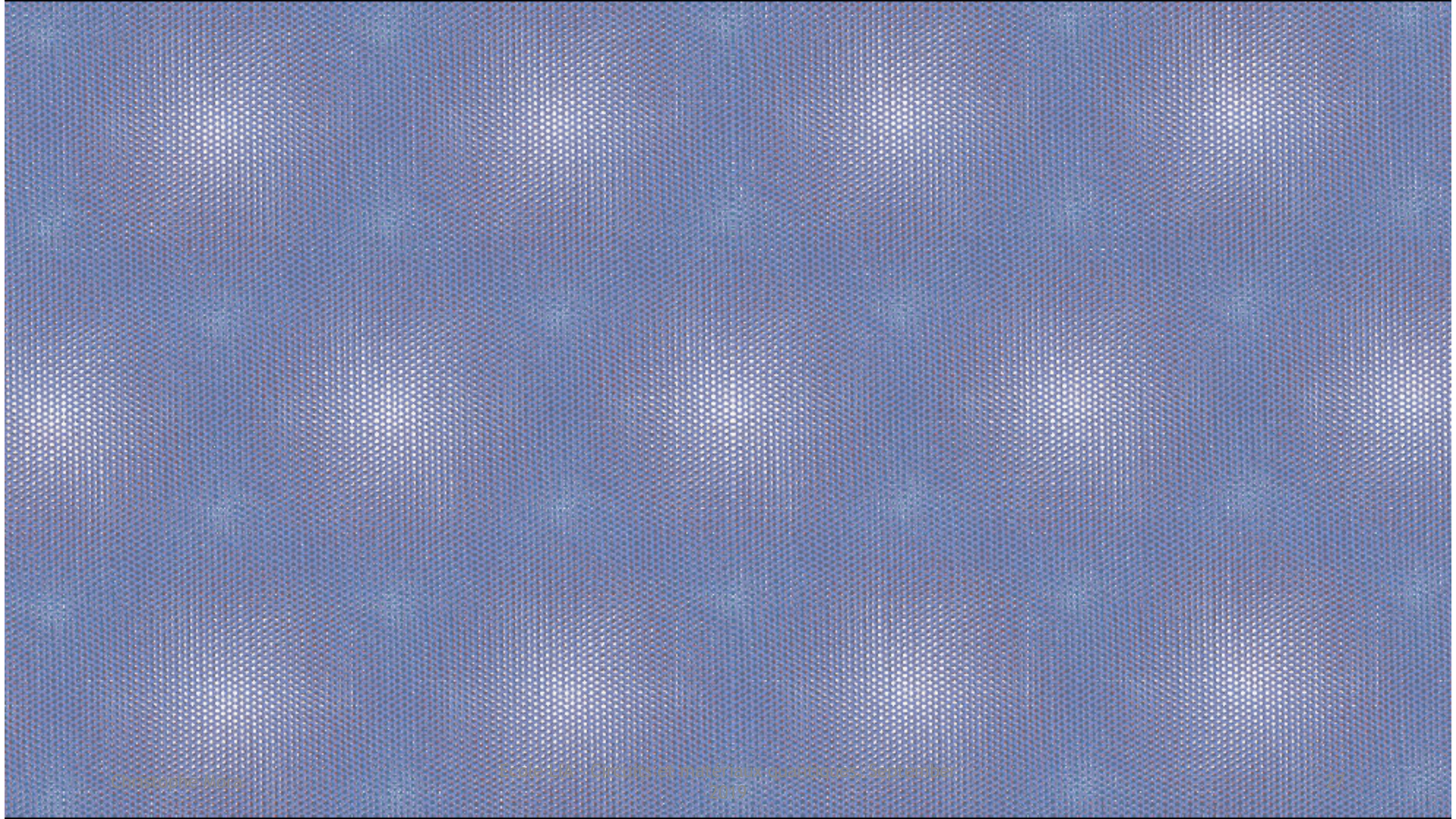
Shifted Dirac cones and flat bands

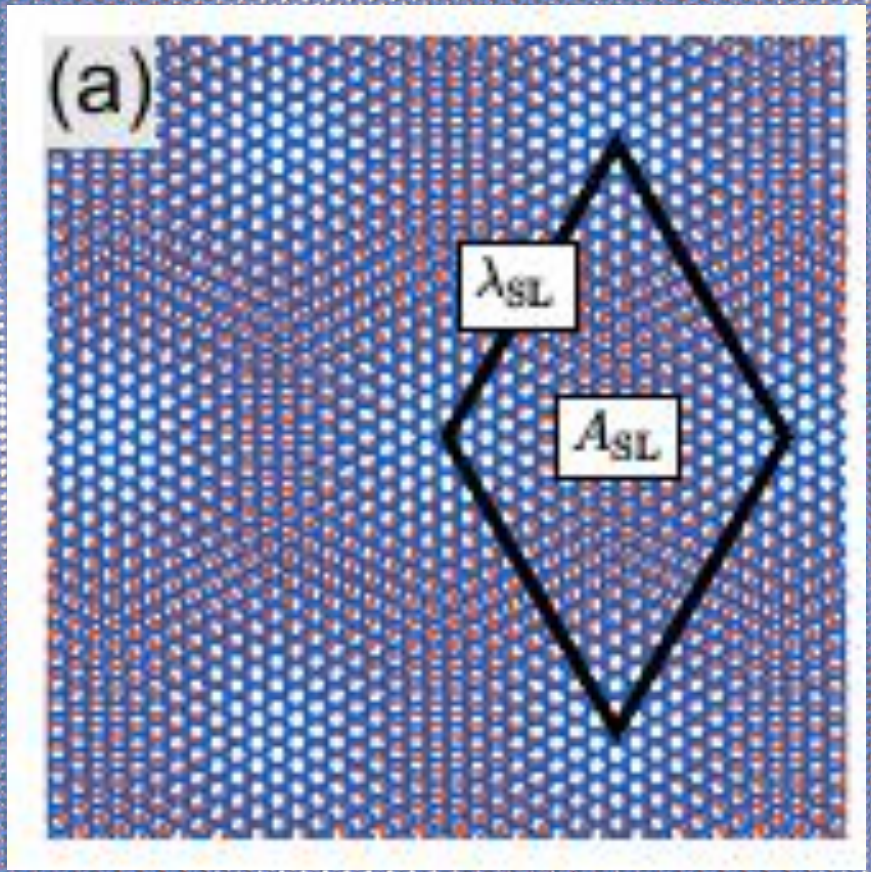




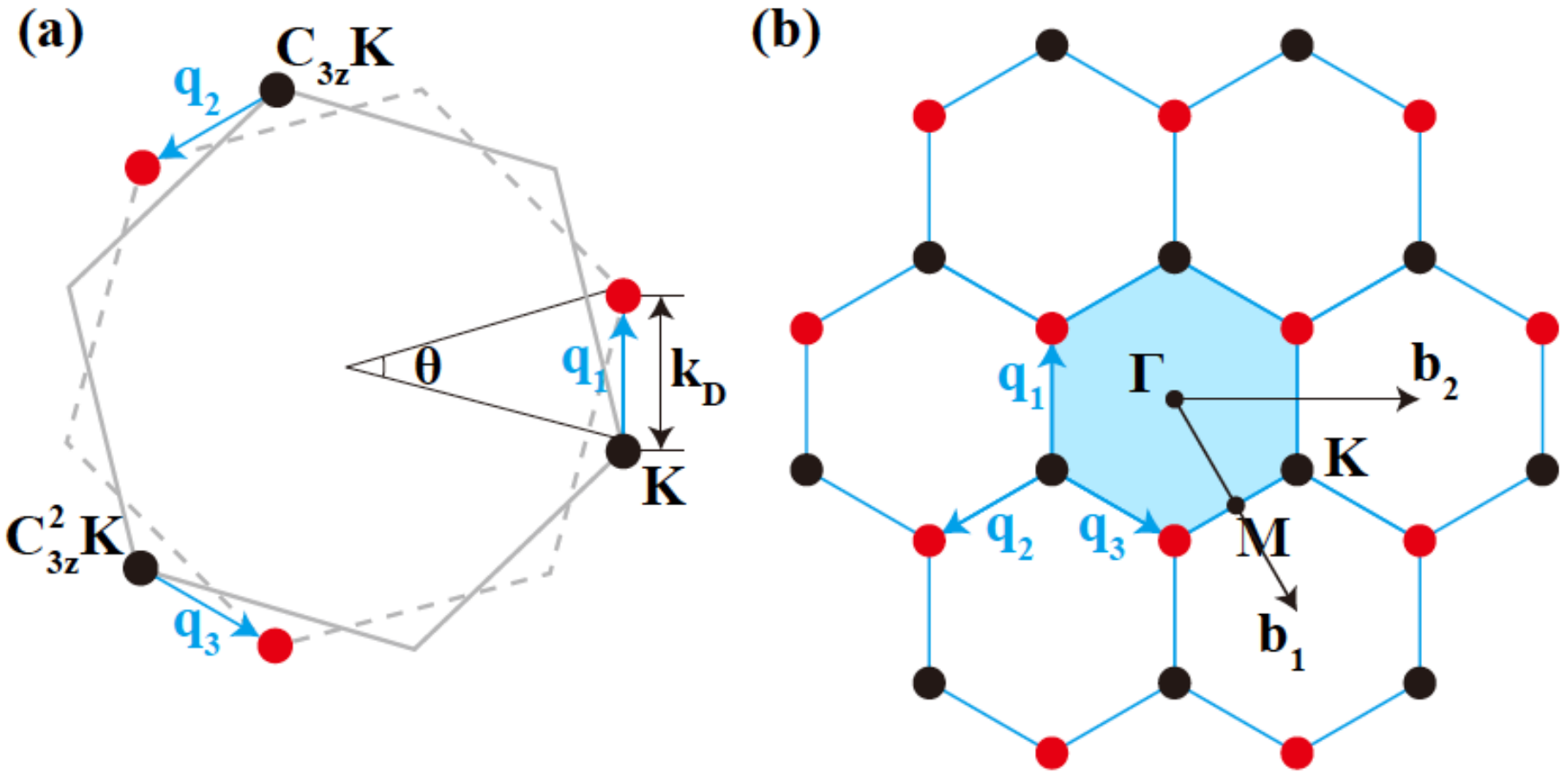
T. Heikkilä & T. Hyart 2019



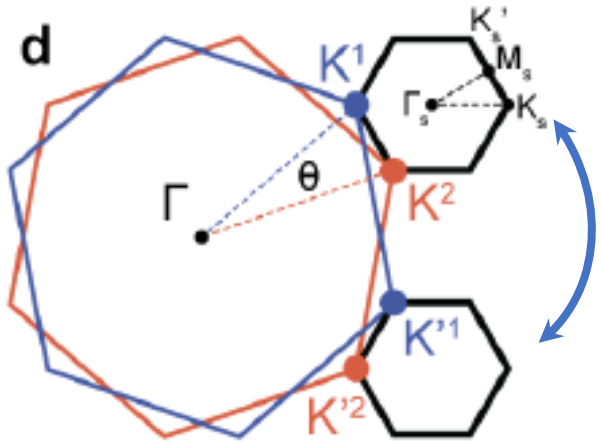



(a)
λ_{SL}
A_{SL}

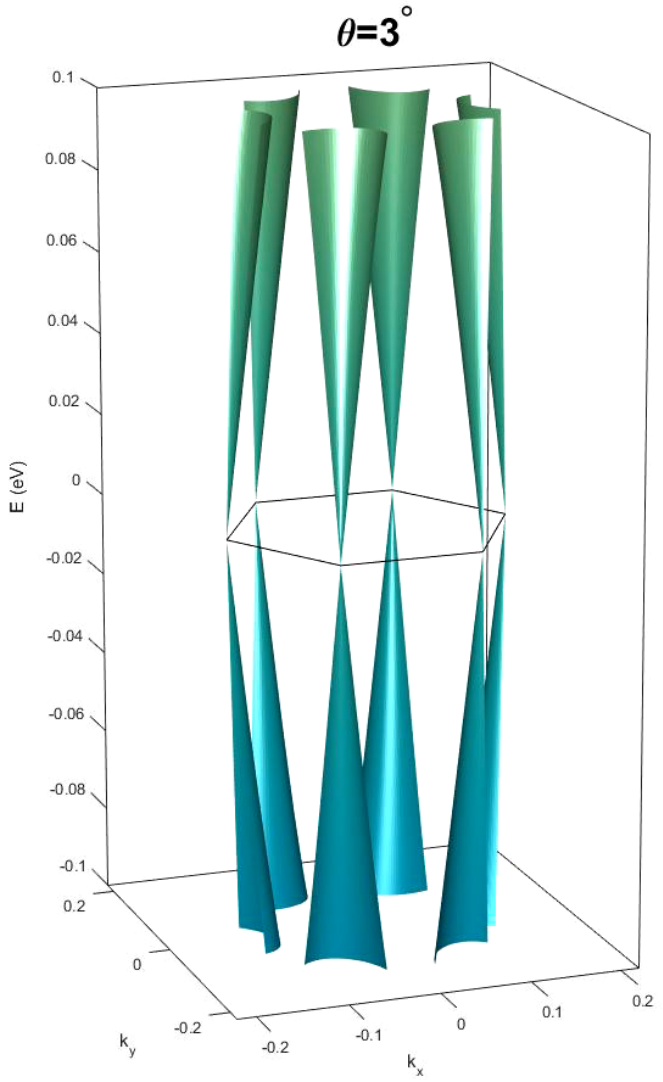
Moiré Brillouin zone



Moiré Brillouin zones

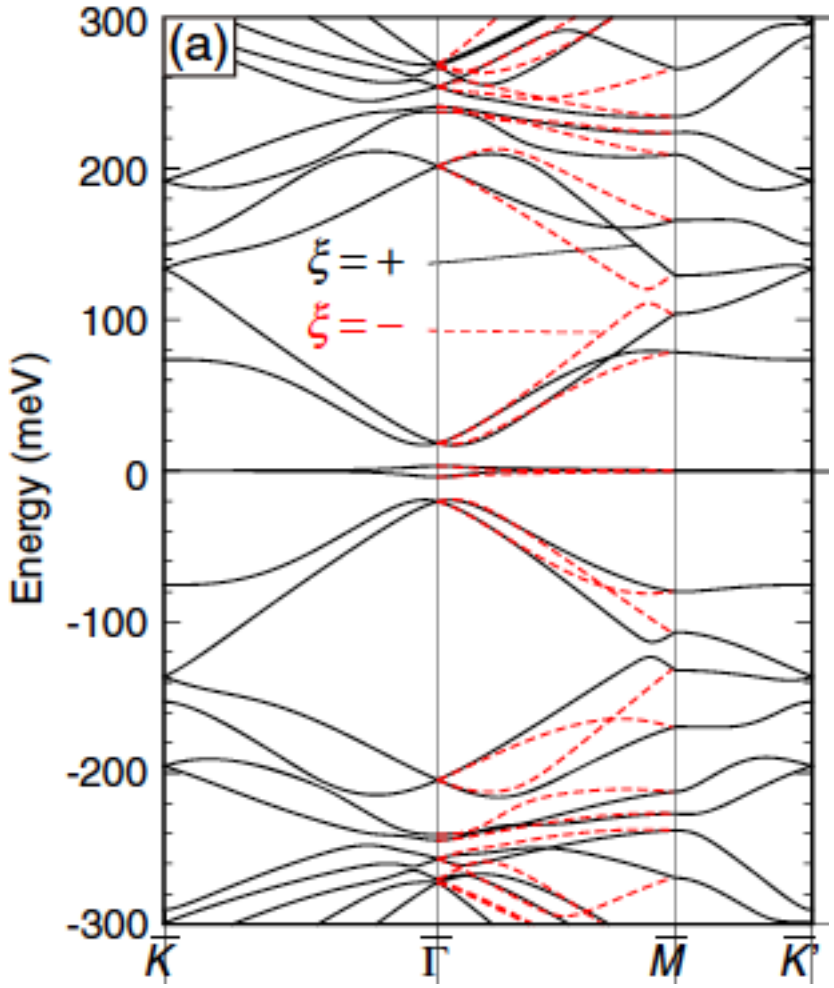


Valley decoupling at small angle

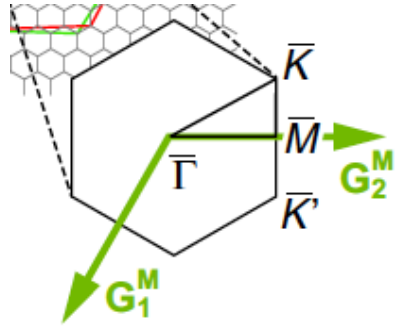


Jarillo-Herrero, Kaxiras, 2018

Two narrow bands close to the Fermi energy



$\theta = 1.05^o$



Koshino et al, PRX 2018

Two narrow bands close to the Fermi energy

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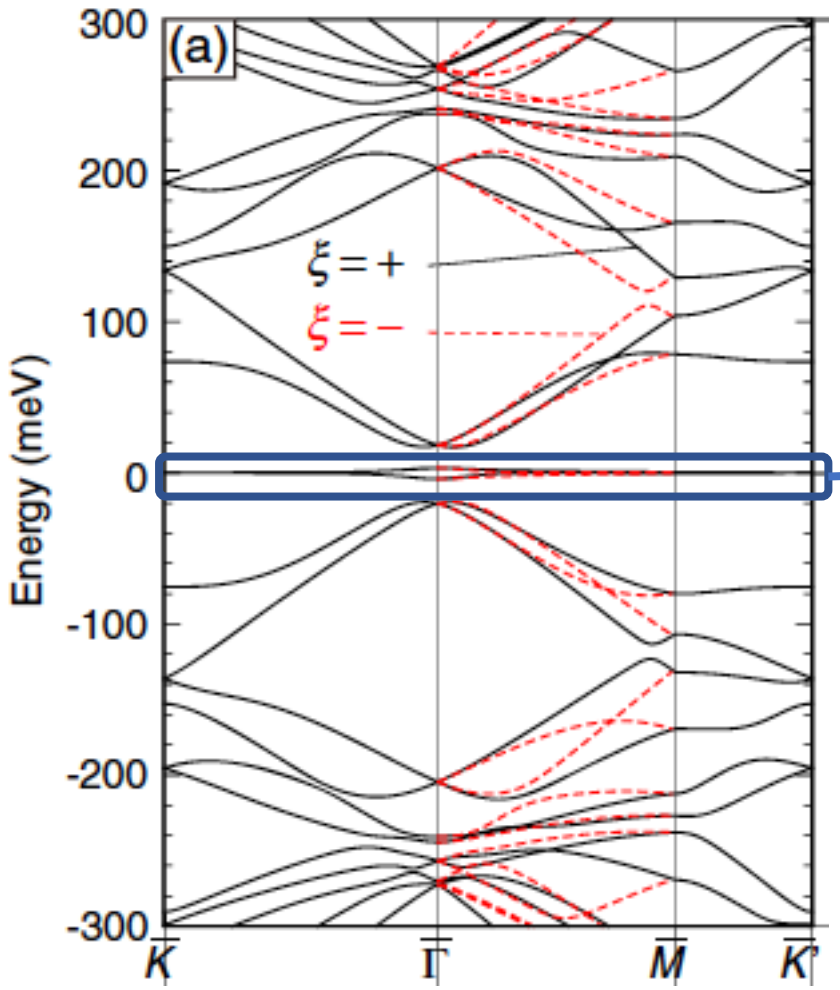
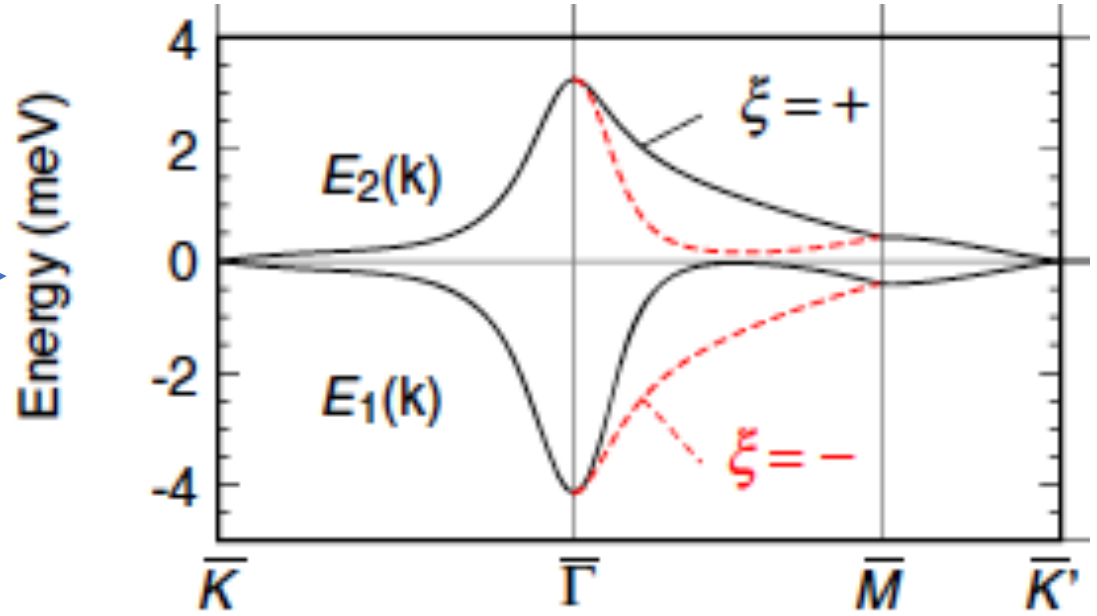
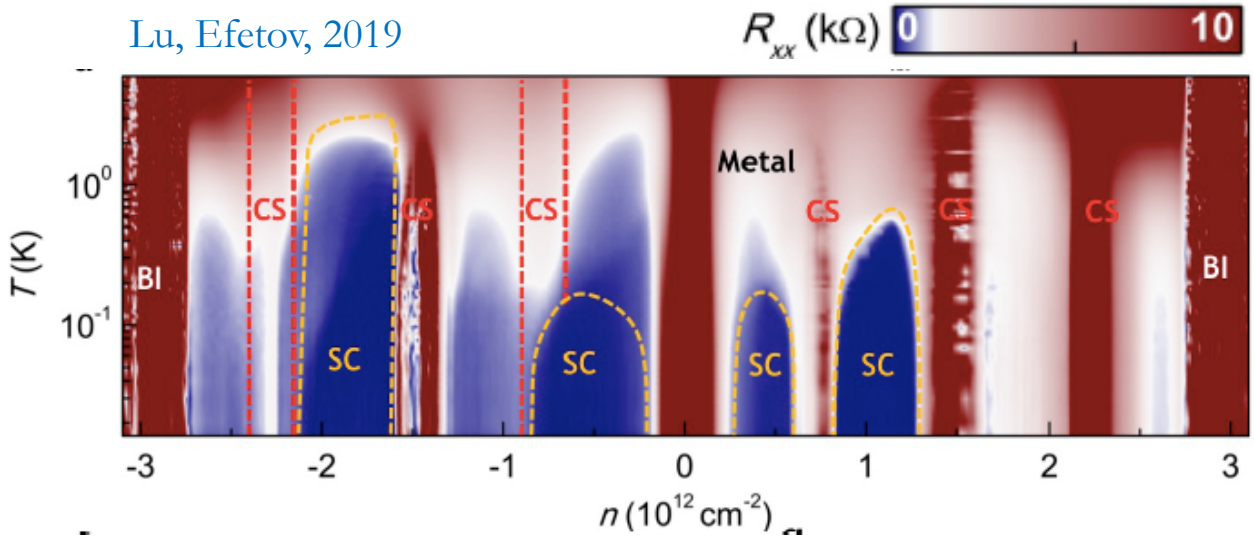




Koshino et al, PRX 2018

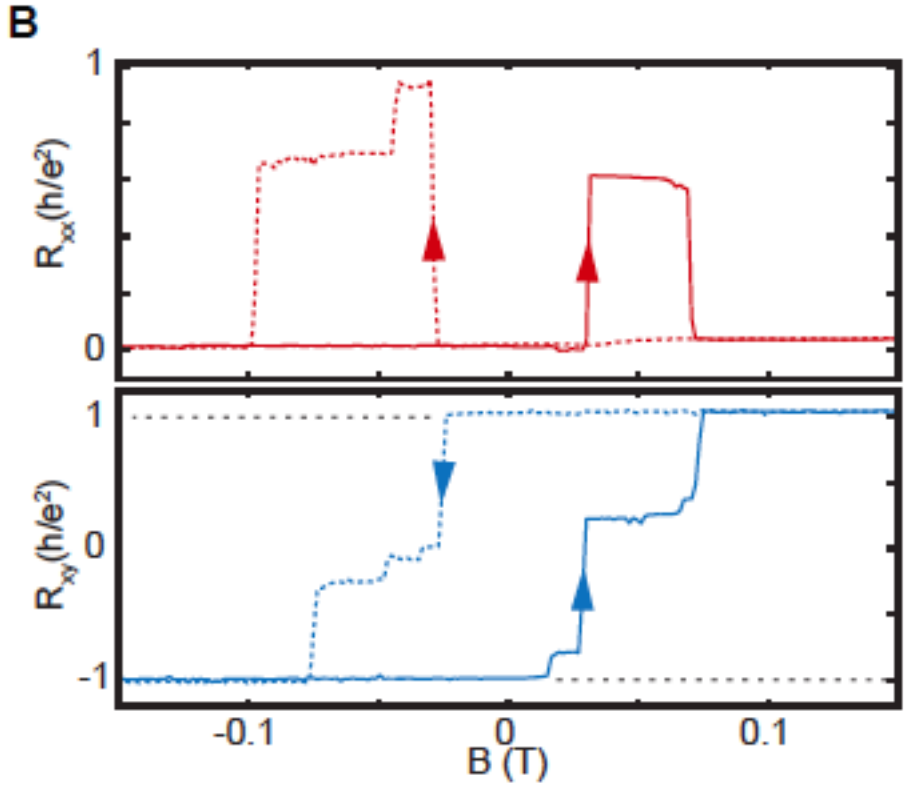
Correlated states

Lu, Efetov, 2019



Multiple correlated and superconducting states

Quantum anomalous Hall effect



Serlin, Young 2019