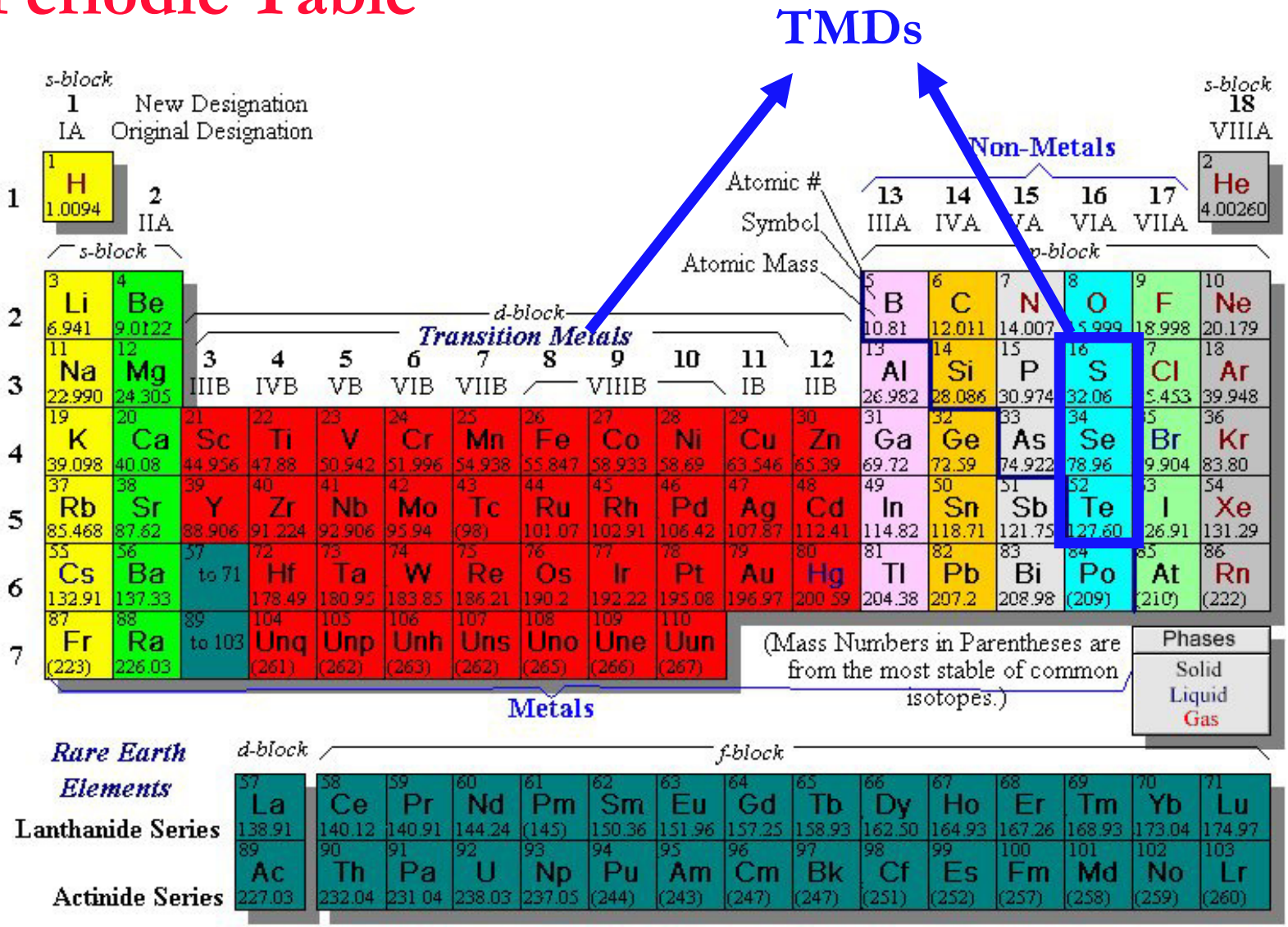
In This Lecture:

- Two-dimensional Materials:

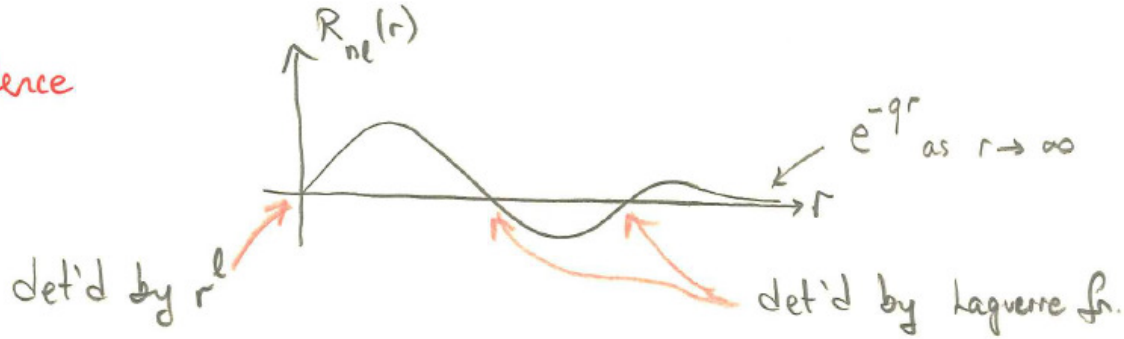
Transition Metal Dichalcogenides

Periodic Table

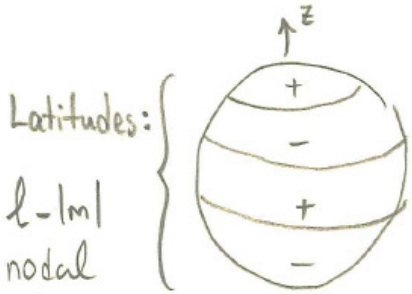


Orbital Profiles: $R_{nl}(r)\ Y_{lm}(\theta,\phi)$

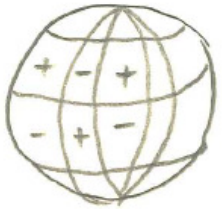
Radial Dependence



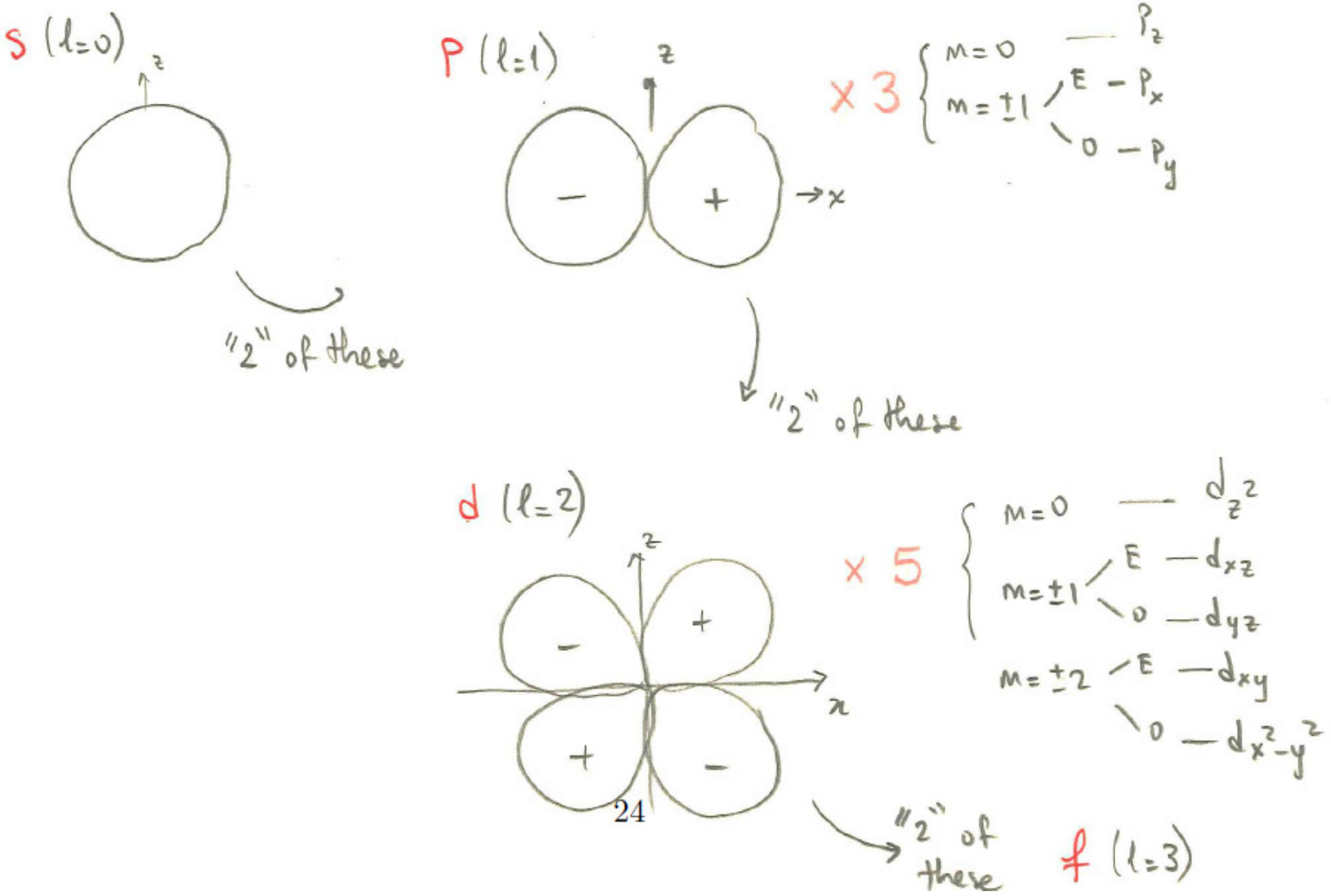
Polar Dependence $P_l^m(\cos\theta)$



Azimuthal Dep. $\sin m\phi,\ \cos m\phi$



$Y_{lm}(\theta,\phi)$: l nodal lines

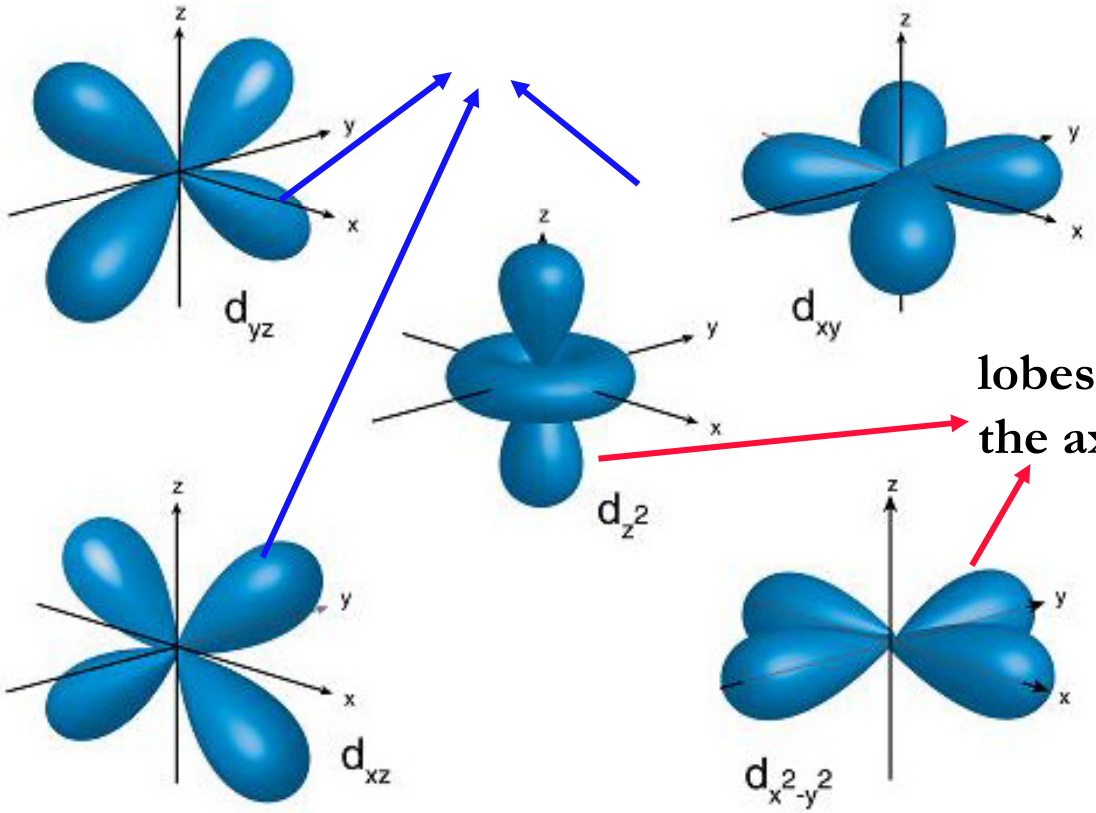

S (l=0)
z
"2" of these
P (l=1)
z
x
−
+
"2" of these
x 3
m=0 — p_z
m=±1 / E − p_x
\ 0 − p_y
d (l=2)
z
x
−
+
+
−
"2" of these
f (l=3)
x 5
m=0 — d_{z^2}
m=±1 / E — d_{xz}
\ 0 — d_{yz}
m=±2 / E — d_{xy}
\ 0 — $d_{x^2-y^2}$

d-orbital electronics

Mo: [Kr]. $5d^5.6s^1$
W: [Xe].$4f^{14}.5d^4.6s^2$

New in se/c's

orbitals lie in the x-y, x-z, and the y-z planes (but not along any of the axes)

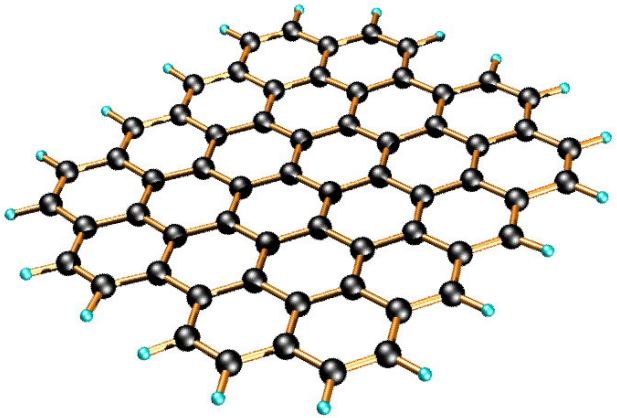


lobes aligned with the axes

Source: socratic.org

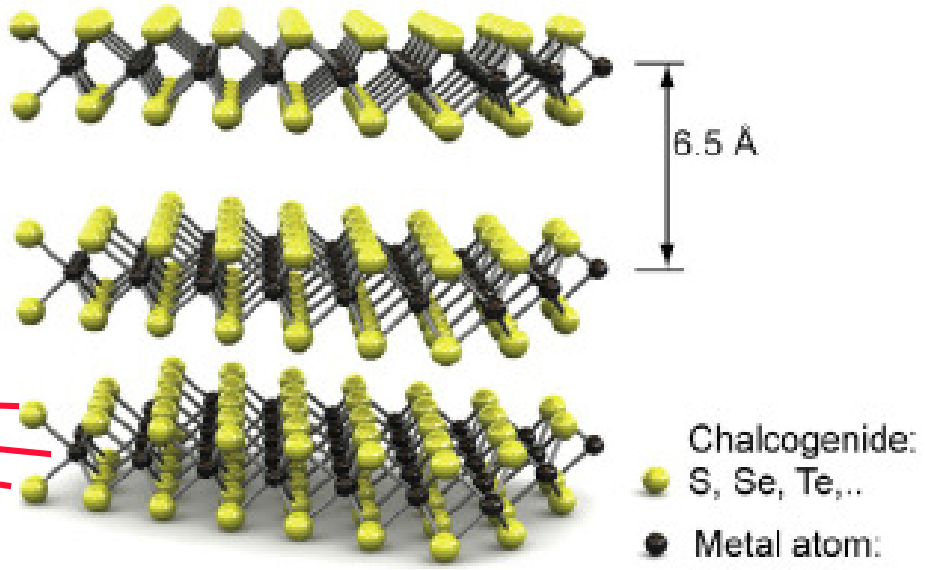
Graphene versus TMDs

Graphene → single sheet



Source: cnx.org

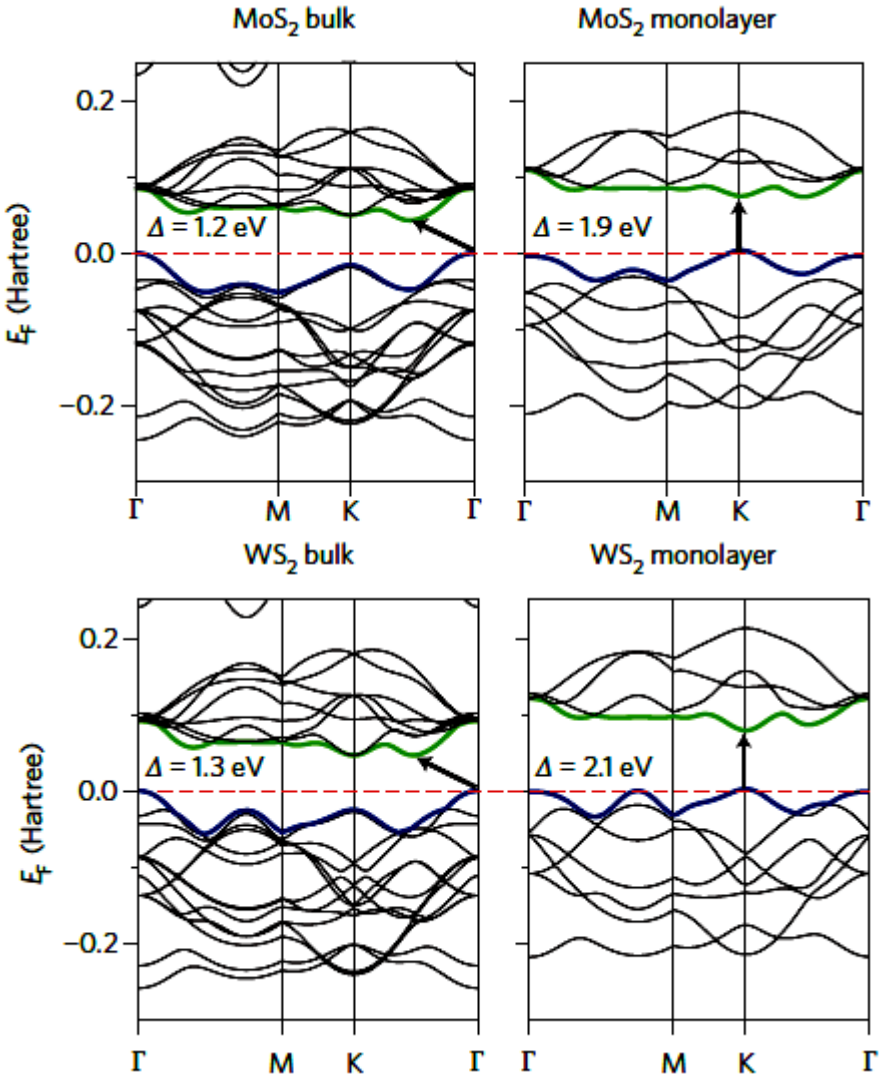
TMD MX_2 → multilayer/monolayer



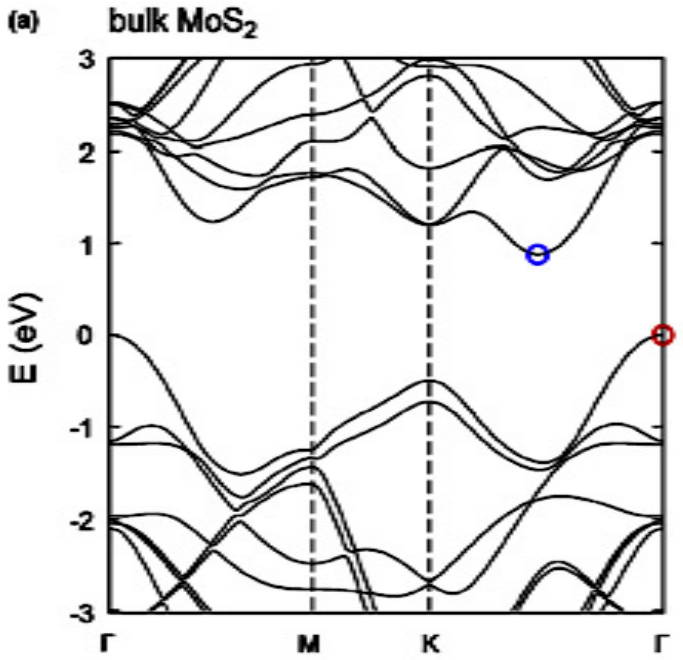
three sheets

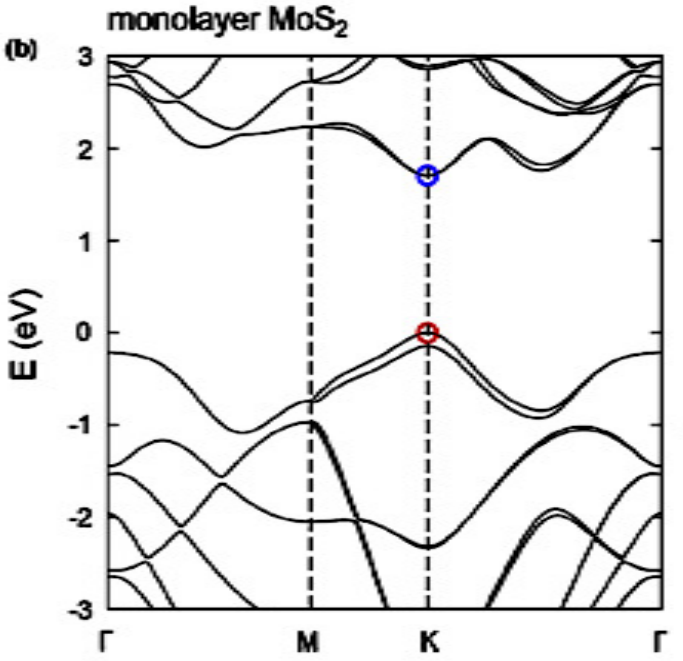
Source: Yazyev Materials Today 2015

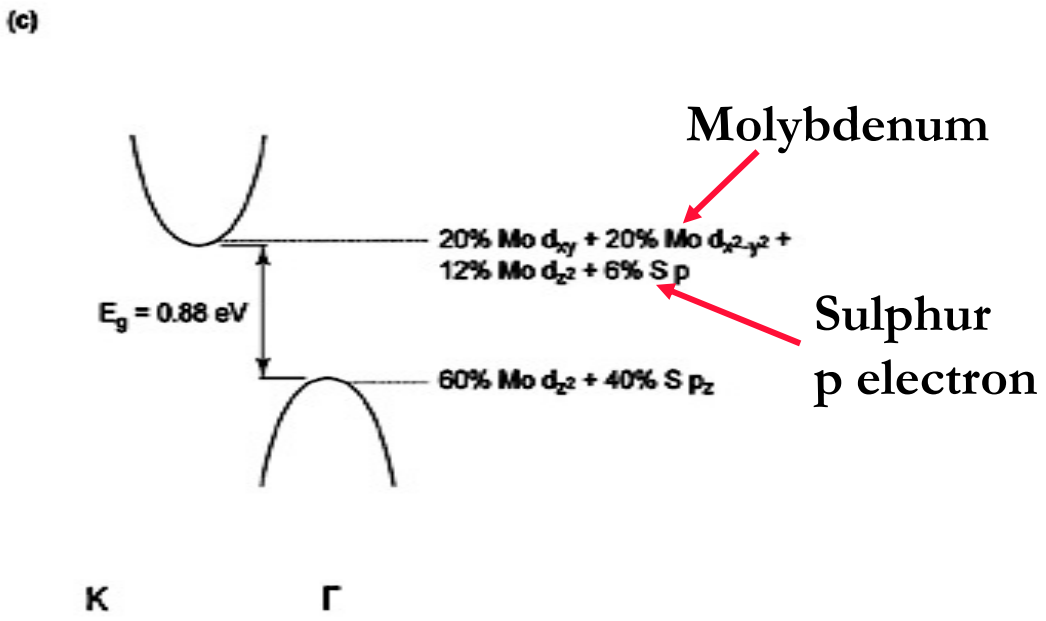
TMDs: bulk vs monolayer

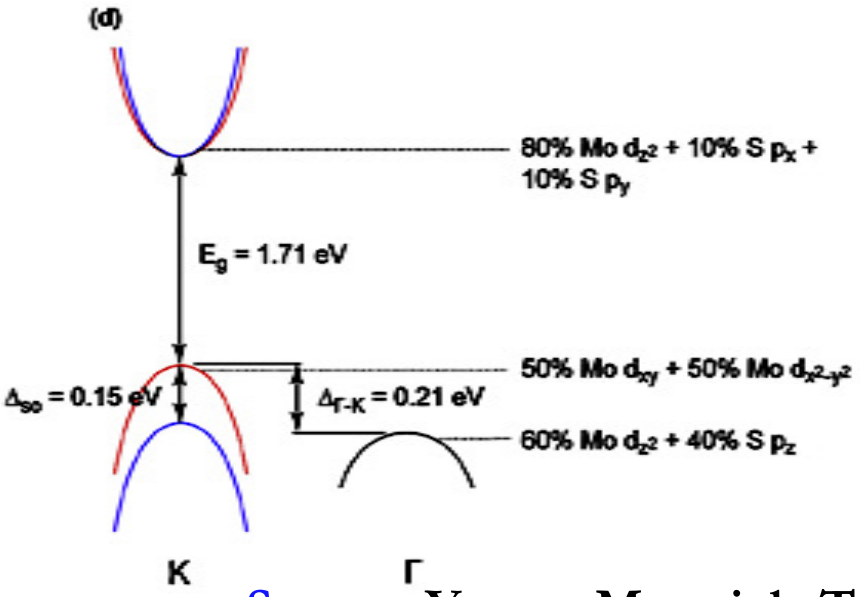


Source: Wang et al. Nature Nano 2012









Source: Yazyev Materials Today 2015

TMDs: atomic orbitals

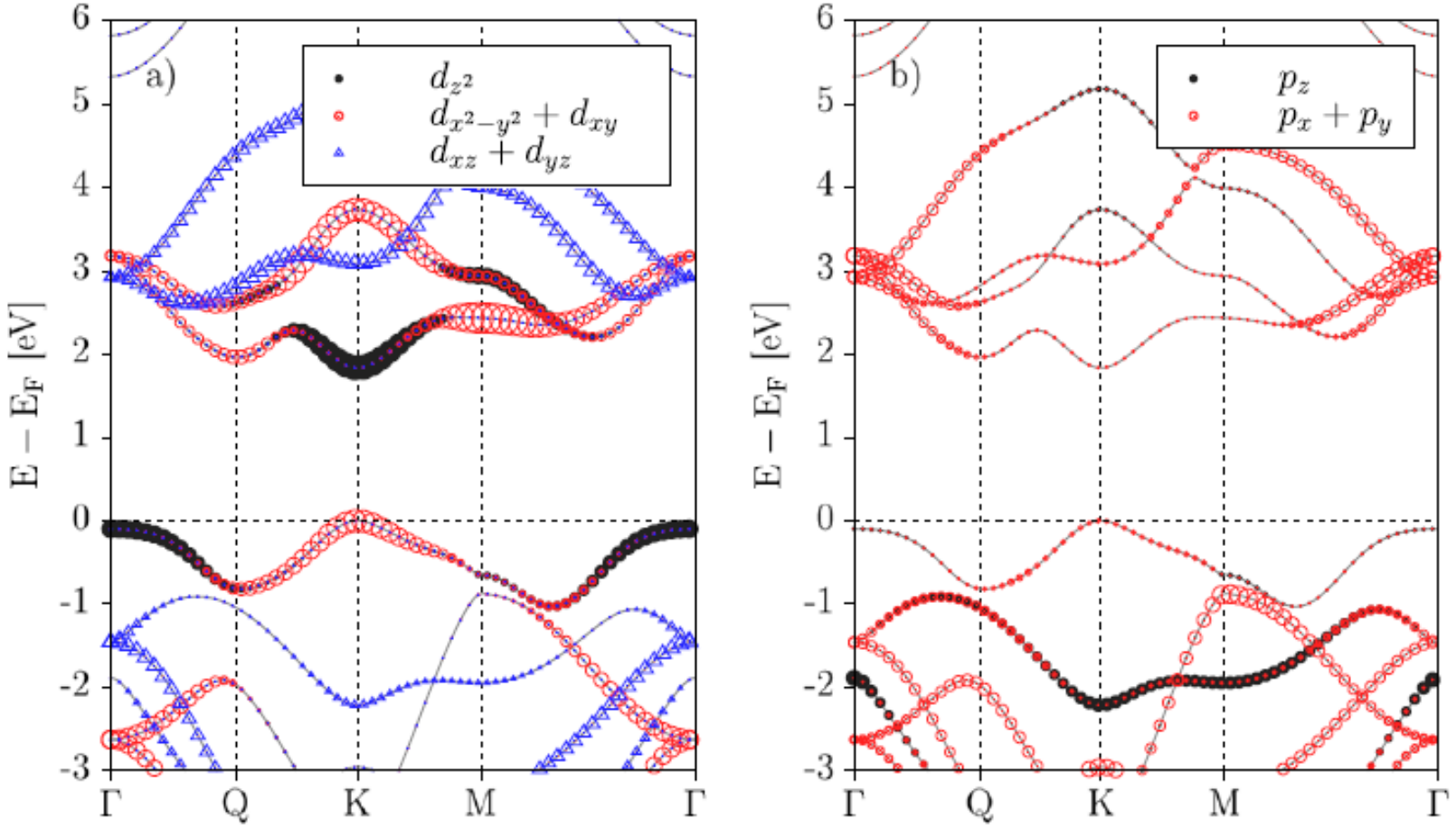


Figure 3. Atomic orbital weights in the energy bands of MX_2. (a) *d* Orbitals of the metal atom, and (b) *p* orbitals of the chalcogen atoms. The size of each symbol is proportional to the weight of the atomic orbital. SOC was neglected in these calculations.

Source: Kormanyos et al. 2D Matl. 2015

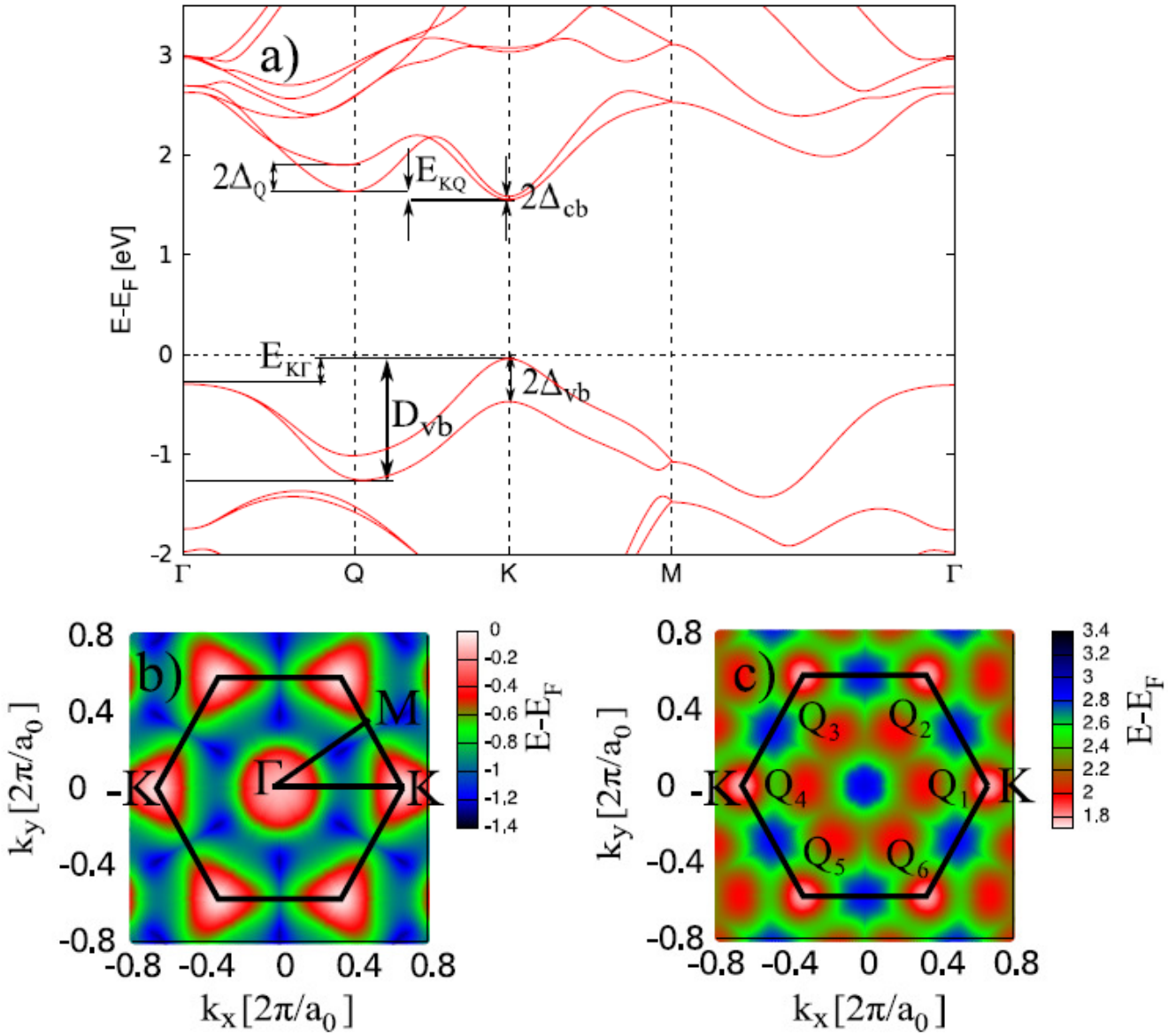
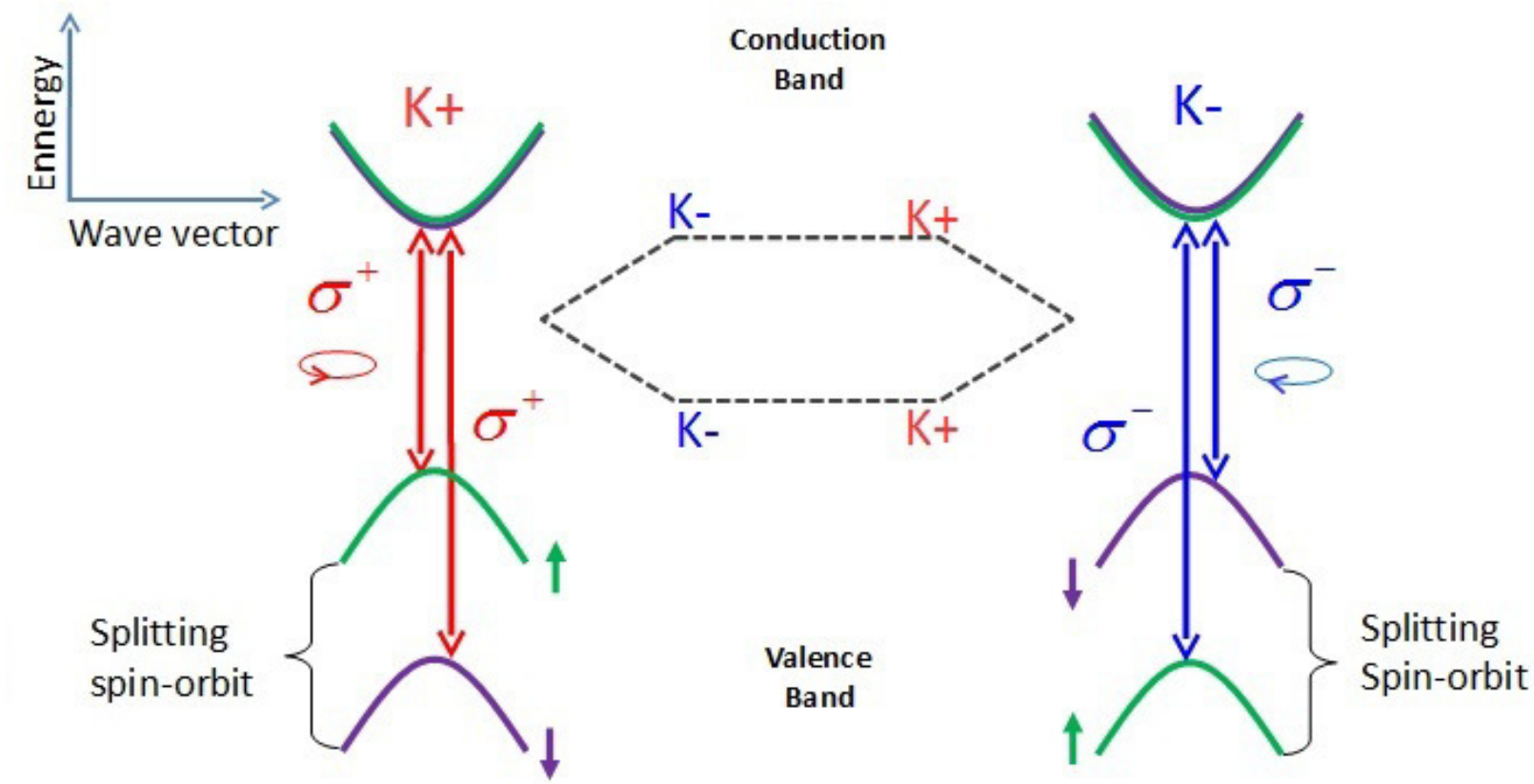


Figure 2. Overview of the band structure of monolayer TMDCs as obtained from DFT calculations. (a) Dispersion along the Γ–K–M–Γ line in the BZ. SOC is taken into account. Various band-edge energy differences and spin-splittings are also indicated; for definitions see the main text. (b) Dispersion of the VB as a function of the wavevector **k** in the whole BZ. The hexagonal BZ is denoted by thick black lines. (c) The same as (b) for the CB. In (b) and (c) SOC is neglected.

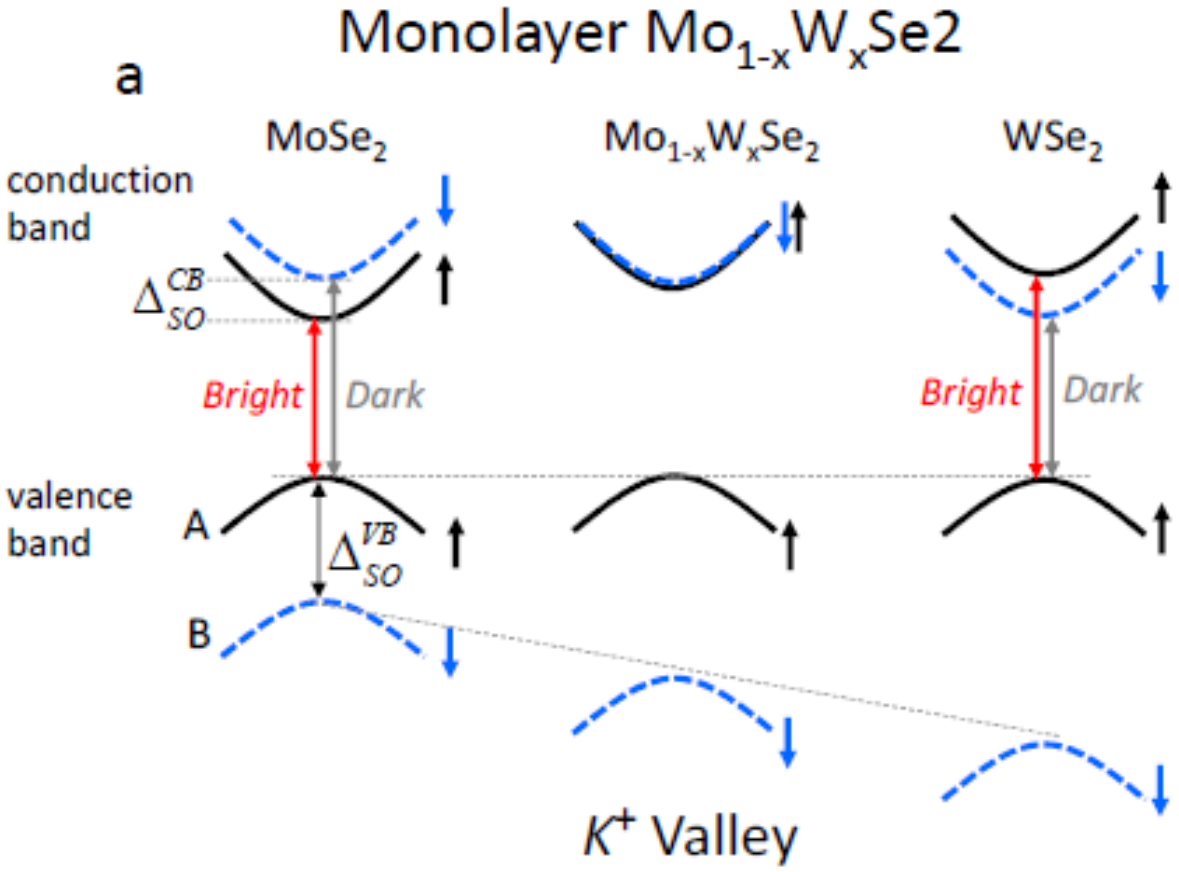
Source: Kormanyos et al. 2D Matl. 2015

Valley Optical Selections



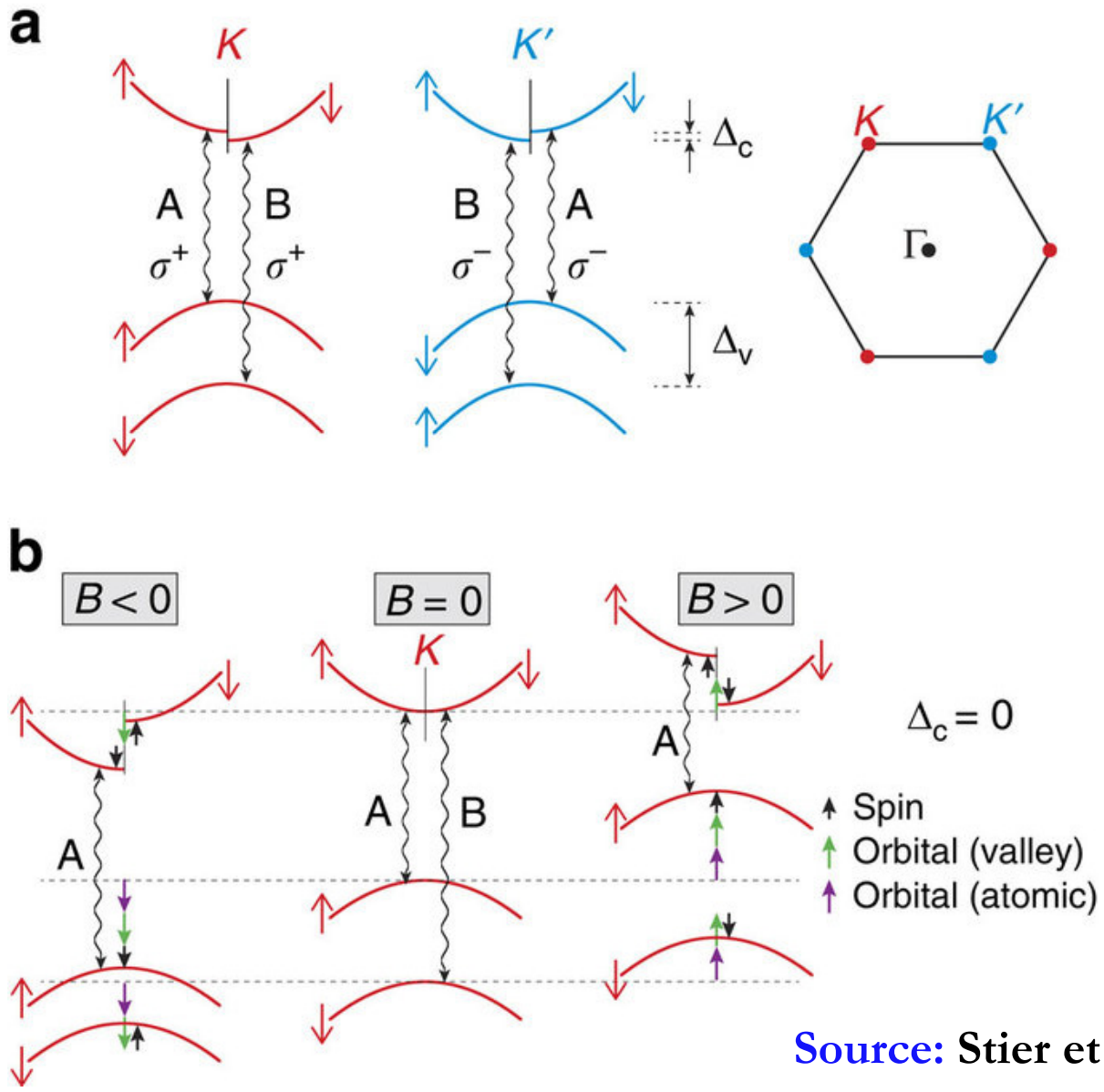
Source: **Wikipedia**

Valleytronics with Alloying



Source: Wang et al. arXiv: 1506.08114

A & B Excitons under Zeeman Effect



Source: Stier et al. Nature Comm. 2016

k.p for TMDs: for $K^{\pm}$ valleys

$$\mathcal{H}_E^{\pm}(q) = \mathcal{H}_1^{\pm}(q) + \mathcal{H}_2^{\pm}(q)\,,$$

$$\mathcal{H}_1^{+}(q) = \begin{pmatrix} E_{v-5} & \delta_7 q_- & \delta_6 q_+ & \delta_4 q_- & 0 & \delta_2 q_+ \\ \delta_7 q_+ & E_{v-4} & \delta_5 q_- & 0 & \delta_3 q_+ & \delta_1 q_- \\ \delta_6 q_- & \delta_5 q_+ & E_{v-3} & \gamma_2 q_+ & \gamma_5 q_- & 0 \\ \delta_4 q_+ & 0 & \gamma_2 q_- & E_v & \gamma_3 q_+ & \gamma_4 q_- \\ 0 & \delta_3 q_- & \gamma_5 q_+ & \gamma_3 q_- & E_c & \gamma_6 q_+ \\ \delta_2 q_- & \delta_1 q_+ & 0 & \gamma_4 q_+ & \gamma_6 q_- & E_{c+2} \end{pmatrix},$$

$$\left[\mathcal{H}_2^{\pm}(q)\right]_{nl} = \frac{\hbar^2 q^2}{2m_n'}\delta_{nl}\,,\quad n,l = 1..6$$

$$q_{\pm} = q_x \pm \mathrm{i}q_y, \quad q^2 = q_x^2 + q_y^2$$

Source: Rybkovksy et al. arXiv: 1610.02695

TABLE III. Parameters of the $k \cdot p$ model as introduced in Eqs. (6), (7). The values of γ_i and δ_i are given in eVÅ, the units of E_i are eV, the effective masses m'_n are given in the units of m_0. Parameterizations are based on TB models listed in footnotes.

	MoS_2 [a]	MoS_2 [b]	MoS_2 [c]	MoS_2 [d]	MoS_2 [e]	$MoSe_2$ [f]	WS_2 [g]	WSe_2 [h]
E_{v-5}	-6.96	-4.50	-4.99	-6.88	-5.20	-4.42	-5.27	-5.14
E_{v-4}	-5.17	-3.83	-4.32	-4.15	-4.66	-3.70	-4.21	-4.02
E_{v-3}	-9.59	-3.49	-3.62	-10.52	-4.18	-3.36	-3.82	-3.67
E_v	-0.97	-0.03	0	0	-0.05	-0.05	0.04	0.02
E_c	0.86	1.77	2.48	2.47	2.44	1.52	2.00	1.69
E_{c+2}	1.91	2.98	4.04	3.96	4.60	2.50	3.36	2.80
γ_2	-5.75	1.62	2.08	-8.00	-0.88	1.50	1.62	1.49
γ_3	4.27	3.39	4.43	5.93	4.65	2.96	3.91	3.43
γ_4	-0.87	-0.92	-2.14	-1.77	-3.05	-0.91	-1.53	-1.44
γ_5	2.57	-2.66	-3.07	3.36	-8.27	-2.44	-3.26	-3.04
γ_6	1.33	0.94	1.52	1.79	0.67	0.84	1.21	1.05
δ_1	3.19	-4.20	-5.14	4.05	-3.80	-3.86	-4.95	-4.52
δ_2	0.80	-0.19	-0.50	1.26	3.55	-0.16	-0.30	-0.29
δ_3	-0.61	2.08	2.53	0.55	-2.63	2.11	2.23	2.25
δ_4	-2.05	0.14	0.02	-2.09	-0.26	-0.06	0.18	-0.06
δ_5	1.74	2.06	2.15	2.28	-0.42	1.79	2.15	1.88
δ_6	1.45	0.69	0.69	2.23	-0.23	0.48	0.32	0.07
δ_7	7.49	4.45	5.05	6.53	3.90	4.81	4.78	5.14
m'_{v-5}	0.87	0.76	0.67	0.85	0.44	0.67	0.64	0.57
m'_{v-4}	1.34	0.83	0.71	2.00	1.22	0.78	0.84	0.80
m'_{v-3}	6.09	6.92	14.00	1.64	0.62	7.69	9.50	12.32
m'_v	-2.81	6.37	3.04	-3.39	1.03	6.58	6.64	7.16
m'_c	-1.96	-1.16	-0.90	-1.33	-0.40	-1.18	-1.02	-1.04
m'_{c+2}	-0.70	-0.60	-0.47	-0.59	-0.36	-0.63	-0.53	-0.55

Source: Rybkovksy et al. arXiv: 1610.02695

k.p for TMDs

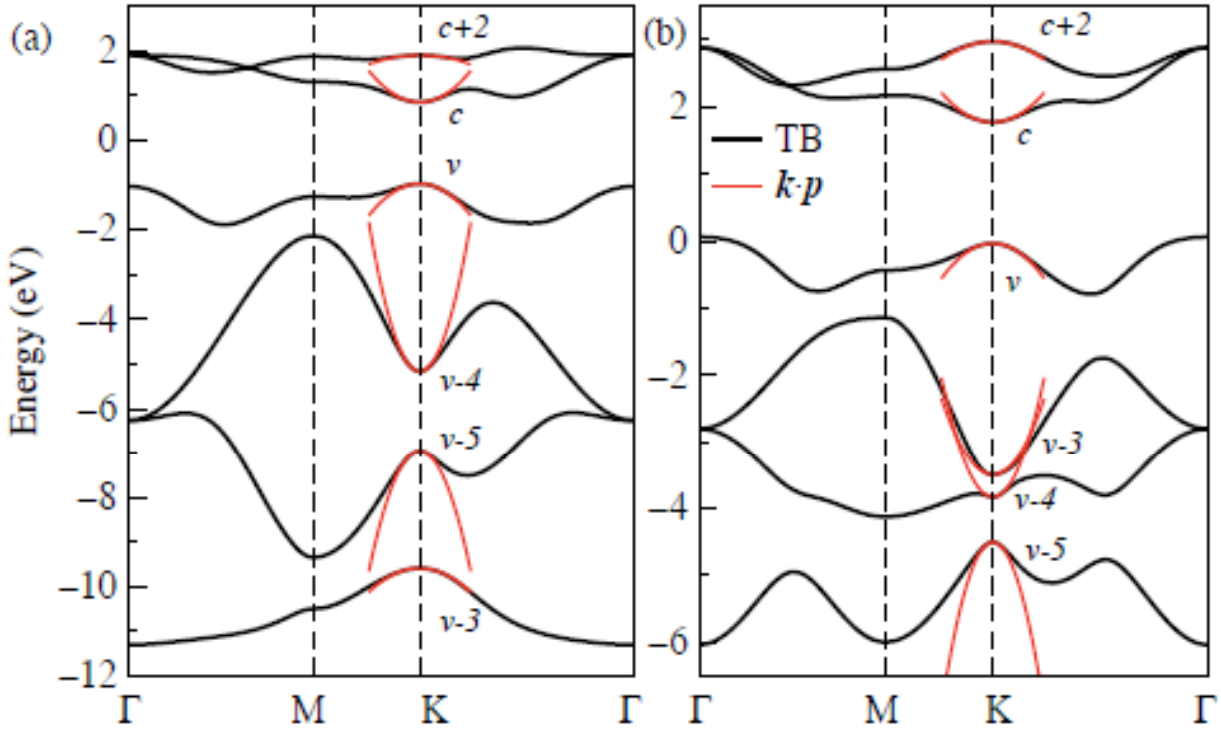


FIG. 1. Electronic spectra of MoS_2 calculated using TB models H. Rostami et al. [26] (a) and S. Fang et al. [24] (b). Red lines are $\boldsymbol{k}\cdot\boldsymbol{p}$ quadratic dispersions at $\boldsymbol{K}$-point calculated using effective masses for each band (see text for details). Note the different order of deep valence bands in two panels.

Source: Rybkovksy et al. arXiv: 1610.02695