Topologické izolátory

ÚFKL
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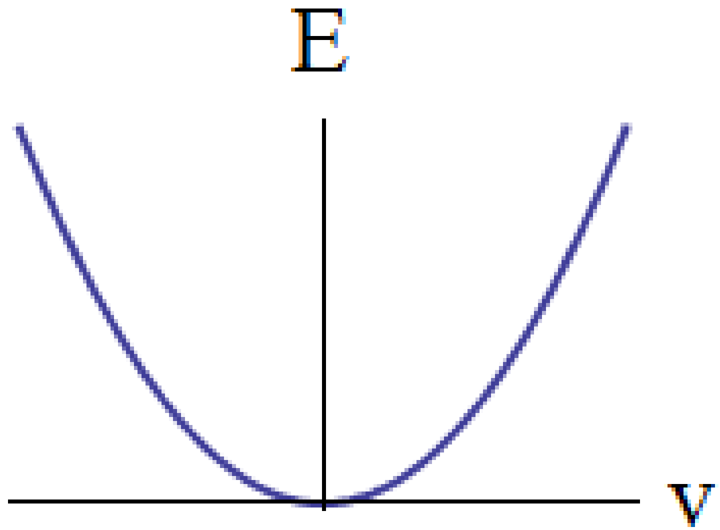
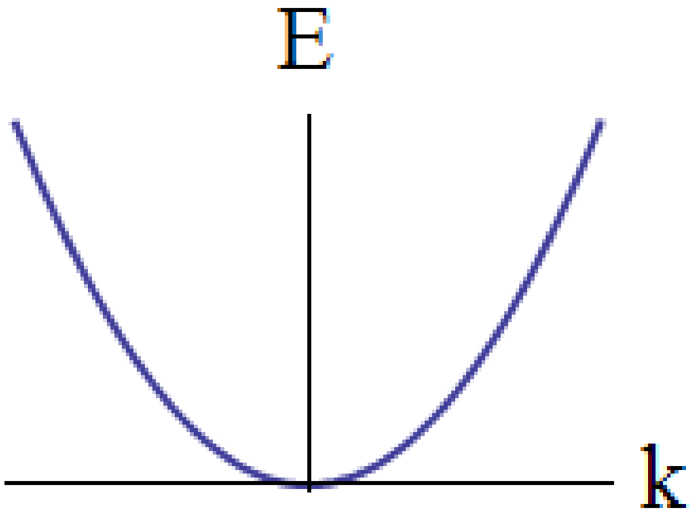
H. Ebert - Uni Mnichov

Osnova

- Krátké a stručné přiblížení pásového modelu pevných látek
- Metody měření pásové struktury
- Topologické izolátory
- Některé experimentální výsledky

Pásová struktura





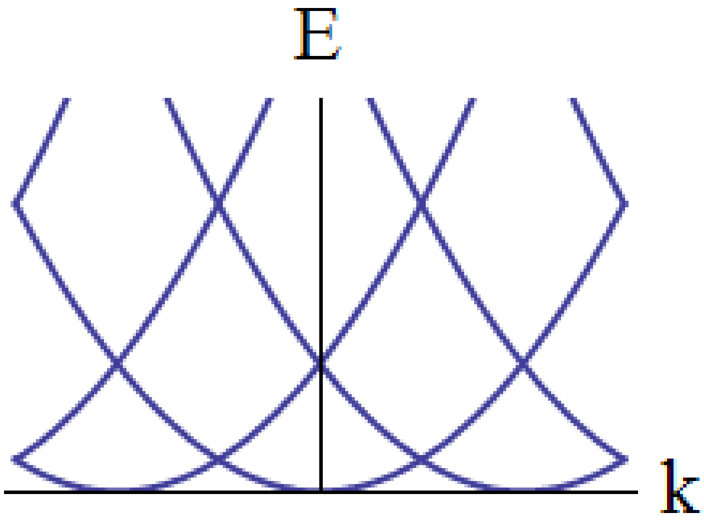
Závislost kinetické energie elektronu na rychlosti

$E=mv^2/2$

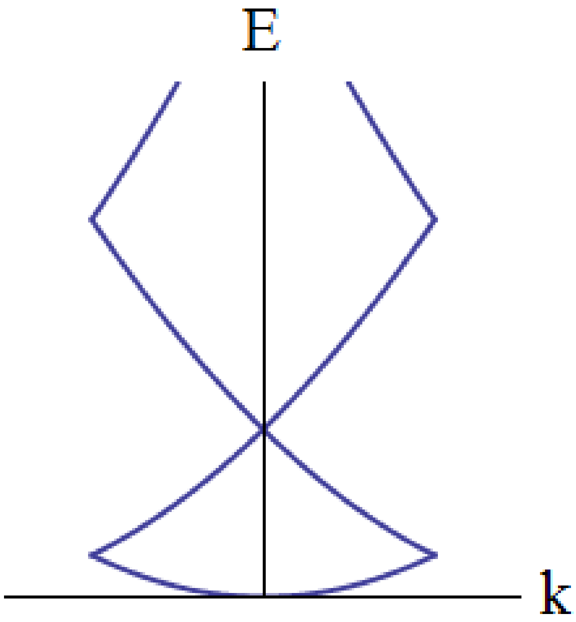
hybnost $p=mv$ $E=p^2/2m$

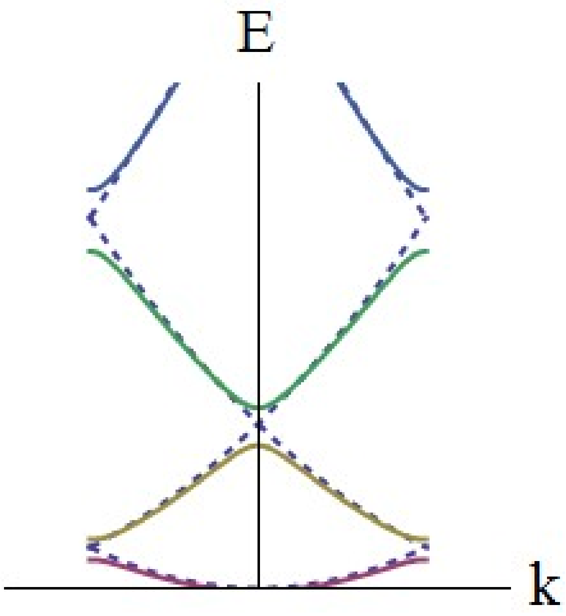
vlnový vektor $p=\hbar k$ $E=\hbar^2k^2/2m$

Pásová struktura



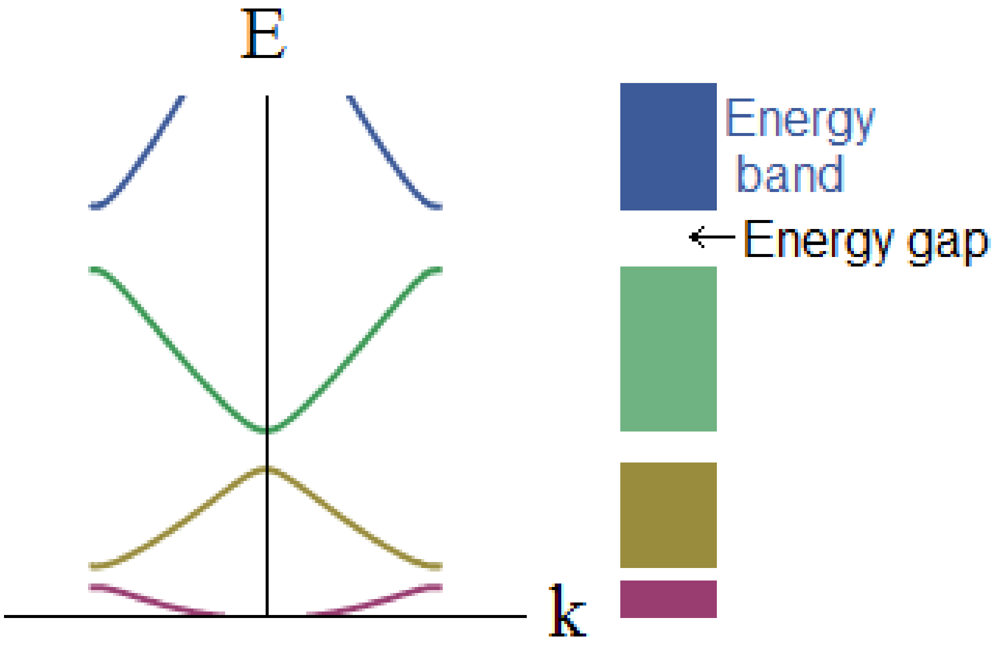
Elektron v krystalové mříži





Vliv elektrostatické interakce s jádry atomů i elektrony navzájem

Pásová struktura



Pásová struktura

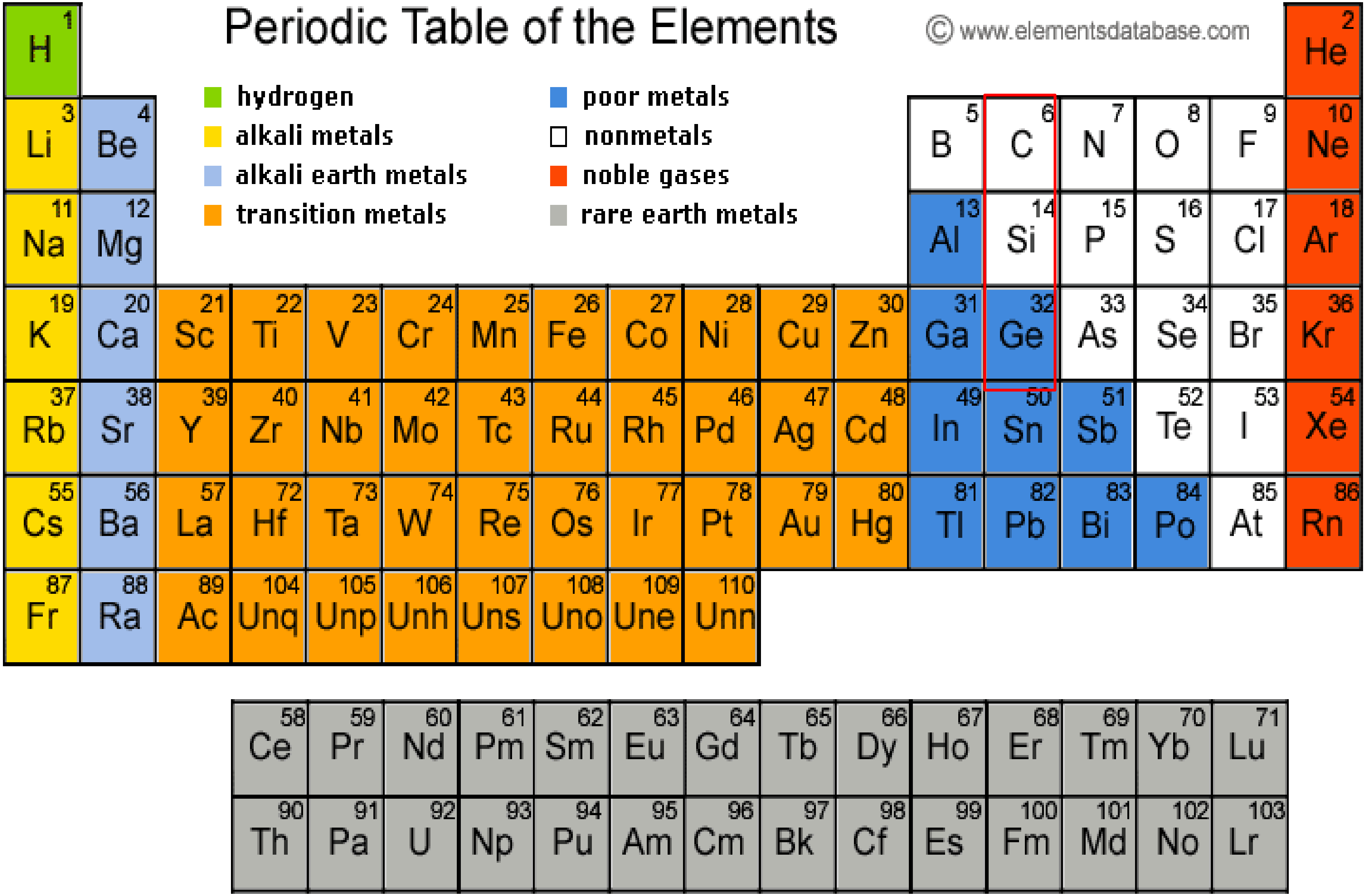
Pauliho vylučovací princip

Kovy: necela zaplněný pás snadná vedení proudu

Zcela zaplněný pás izolátory a polovodiče.

Polovodiče mají zakázaný pás relativně úzký (do cca 4eV), možnost teplné excitace elektronů, dopovaní

Pásová struktura



Periodic Table of the Elements

© www.elementsdatabase.com

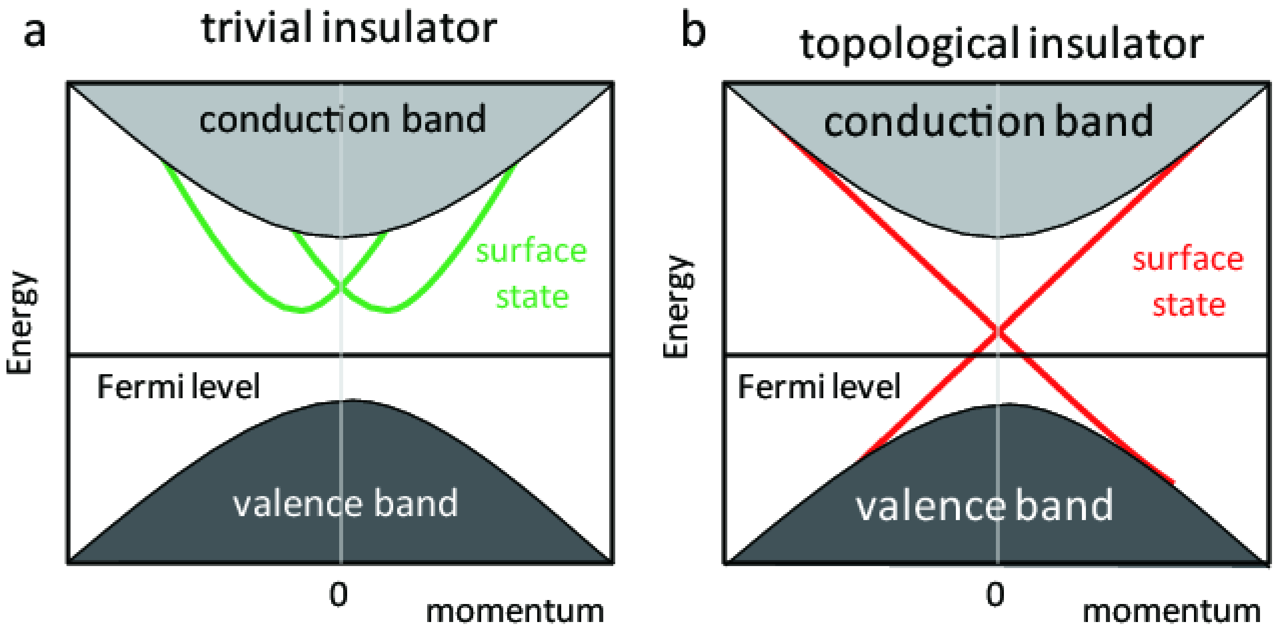
- 🟩 hydrogen
- 🟨 alkali metals
- 🟦 alkali earth metals
- 🟧 transition metals
- 🟦 poor metals
- ☐ nonmetals
- 🟥 noble gases
- ▨ rare earth metals

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Unq	105 Unp	106 Unh	107 Uns	108 Uno	109 Une	110 Unn								
			58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
			90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

Topologické izolátory

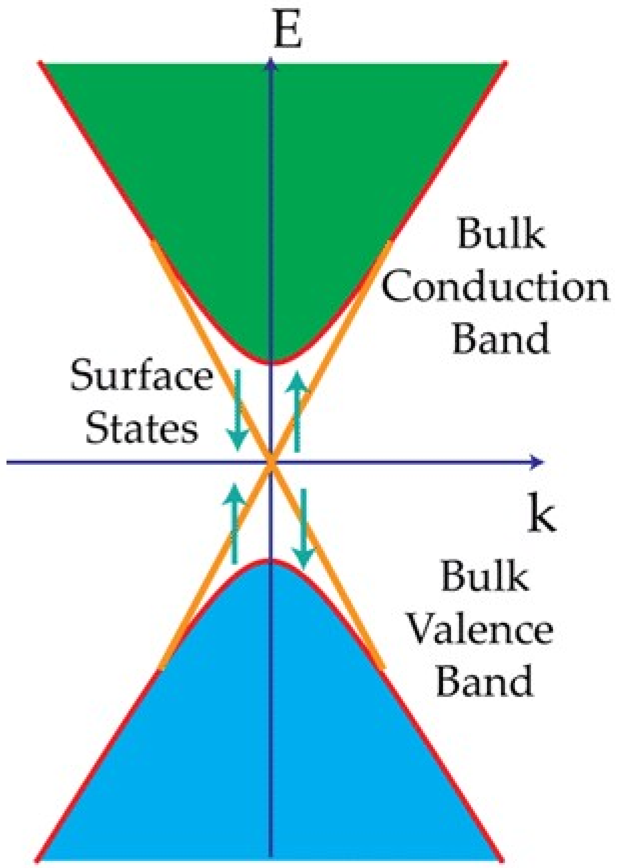
Pásová struktura topologického izolátoru

Povrchové stavy polarizovaného spinu



Topologické izolátory

Pásová struktura topologického izolátoru



Povrchové stavy polarizovaného spinu

Topologické izolátory

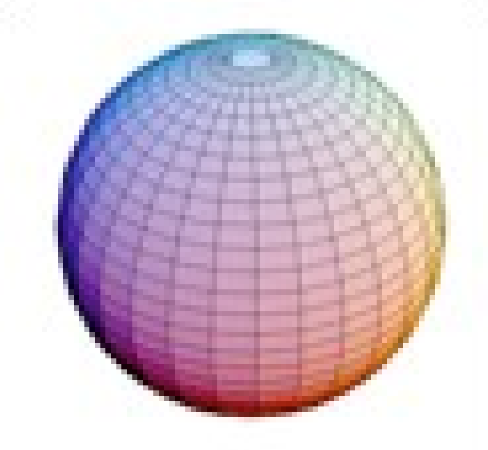
Topologie

Gaussův-Bonnetův teorém

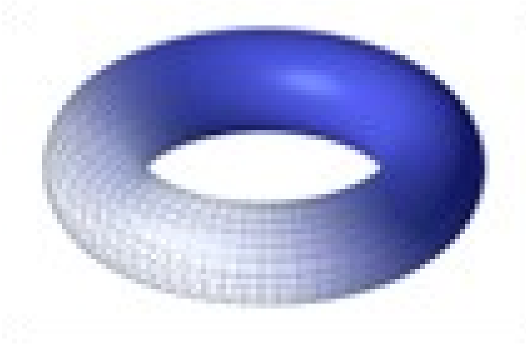
$\kappa = (r_1 r_2)^{-1}$

$$\int_M \kappa \, dA = 2\pi\chi = 2\pi(2-2g)$$

g je genus - “počet děr”



g=0



g=1

Topologické izolátory

V pásové struktuře

$$\psi(\mathbf{r}) = e^{i\mathbf{k}.\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

$$A = \left\langle u_{\mathbf{k}} \middle| -i\nabla_k \middle| u_{\mathbf{k}} \right\rangle$$

$$F = \nabla \times A$$

Berryho křivost

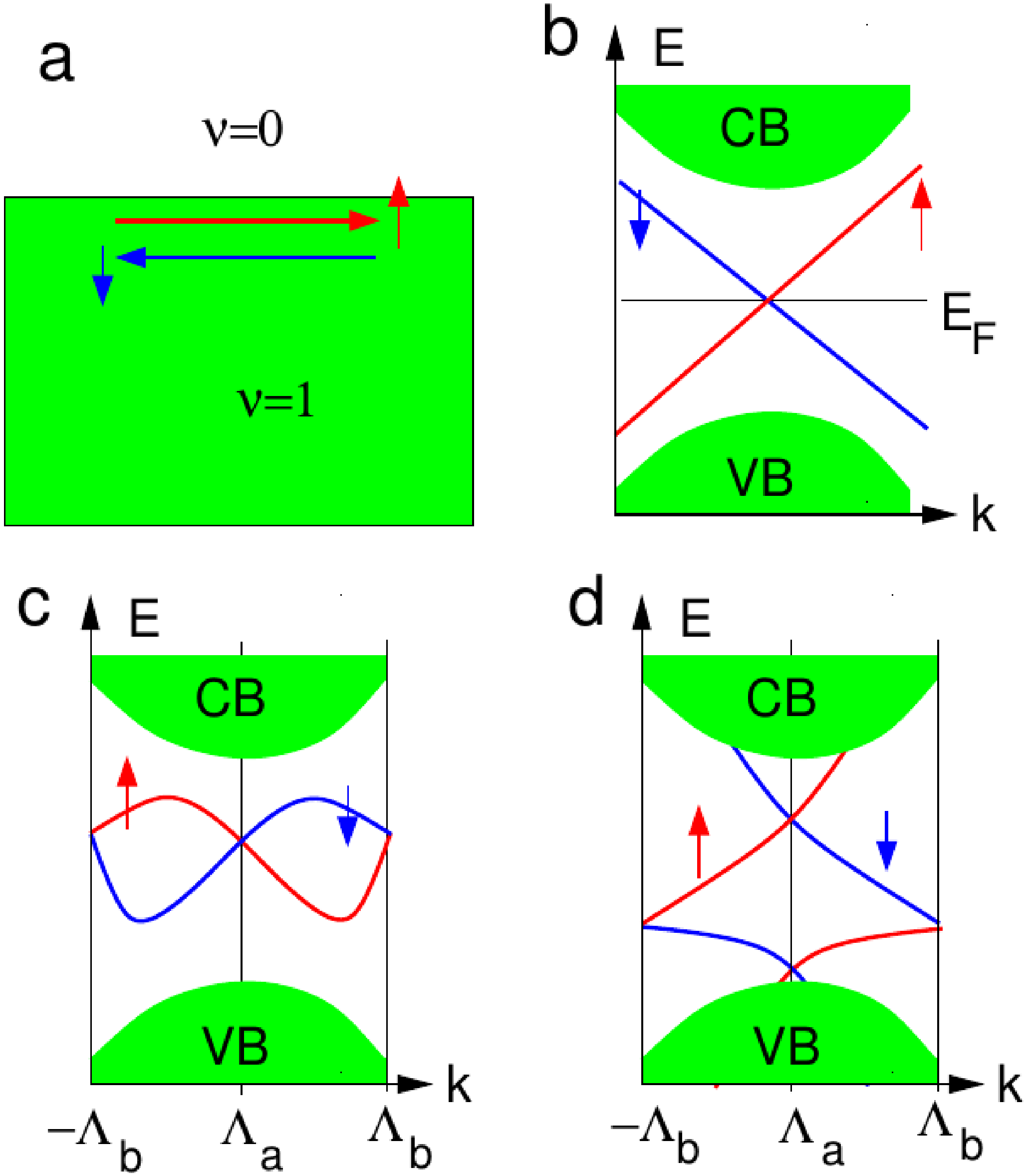
Integrál přes obsazené stavy - Chernovo číslo n

Důsledek:
na rozhraní dvou oblastí
s různým Chernovým číslem
musí existovat povrchové
stavy s jistými vlastnostmi,
které nezávisí na stavu
povrchu (defekty apod.)

NC 2016: David J. Thouless, Duncan Haldane a Michael Kosterlitz
“za teoretické objevy topologických fází hmoty a topologických fázových přechodů”

Různé invarianty Z_0, Z_2, atd.
Jiná rodina topologických izolátorů (Pb,Sn)Se, (Pb,Sn)Te

Topologické izolátory



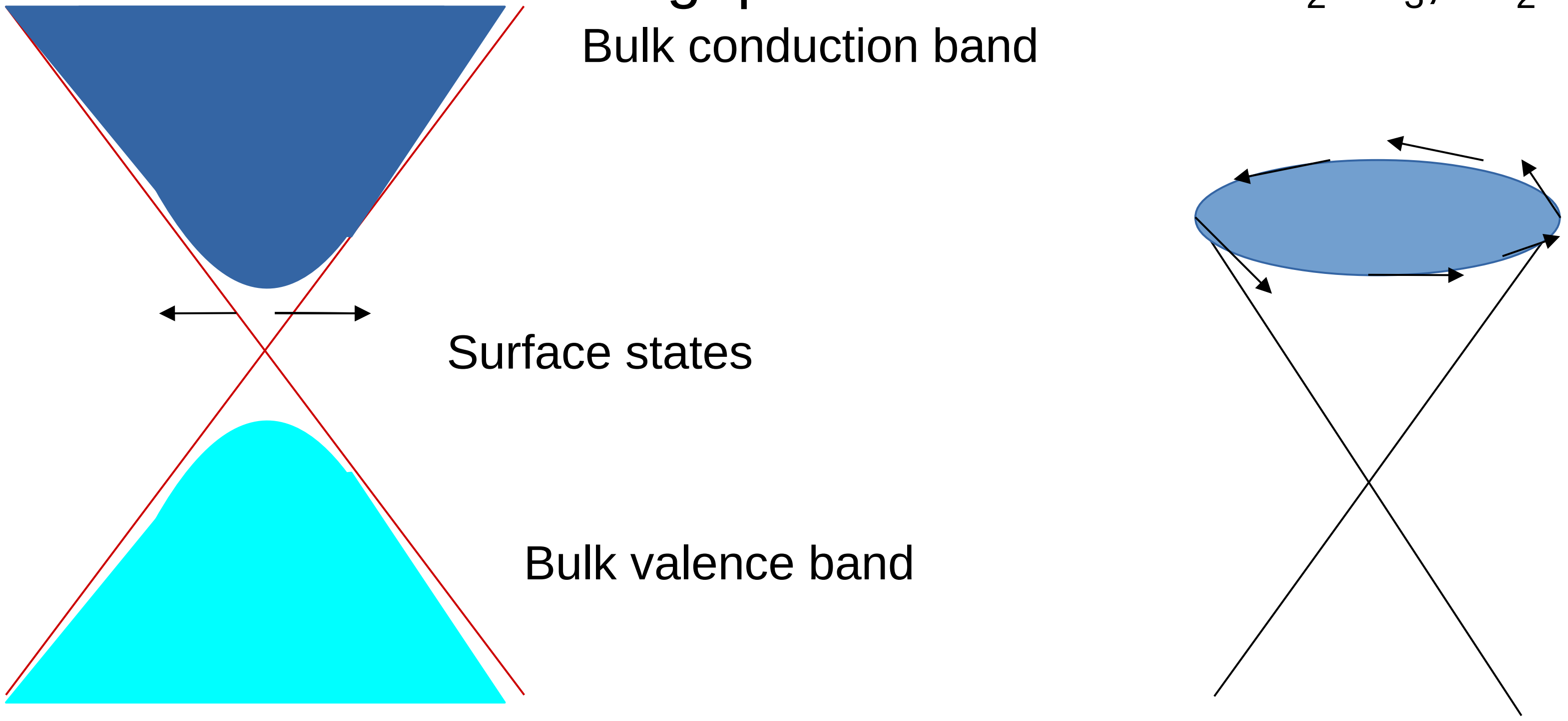
Topological insulators

Band structure of topological insulator:

Large spin orbit splitting and time reversal symmetry

→ spin polarized surface states with Dirac-cone dispersion

Prototypical materials: narrow band gap semiconductors Bi_2Se_3, Bi_2Te_3

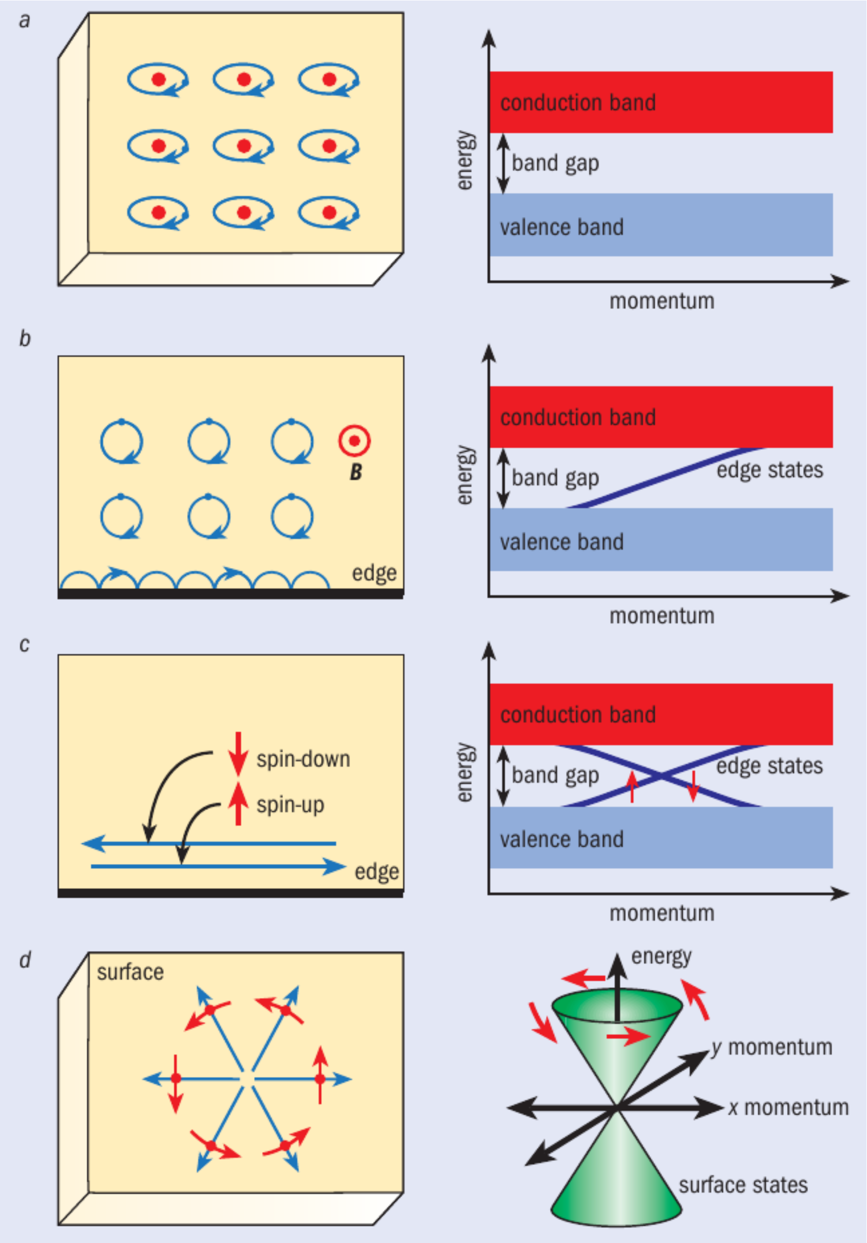


Ferromagnetic ordering brakes time reversal symmetry

→ band gap within surface states, Quantum anomalous Hall effect

Topologické izolátory

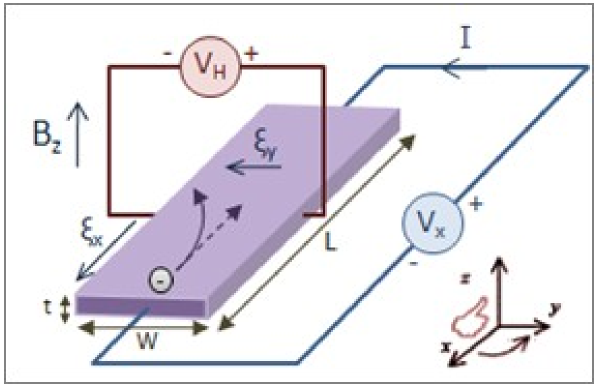
Pásová struktura topologického izolátoru

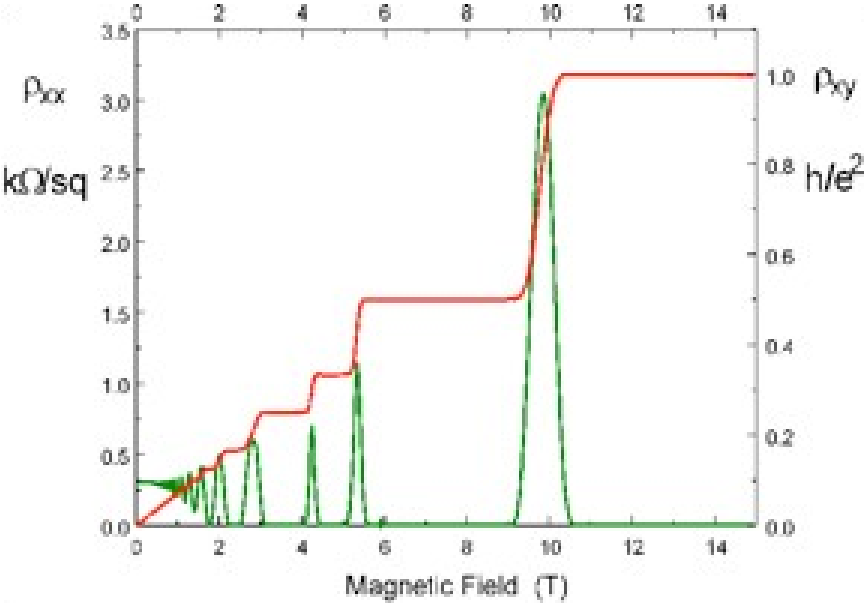


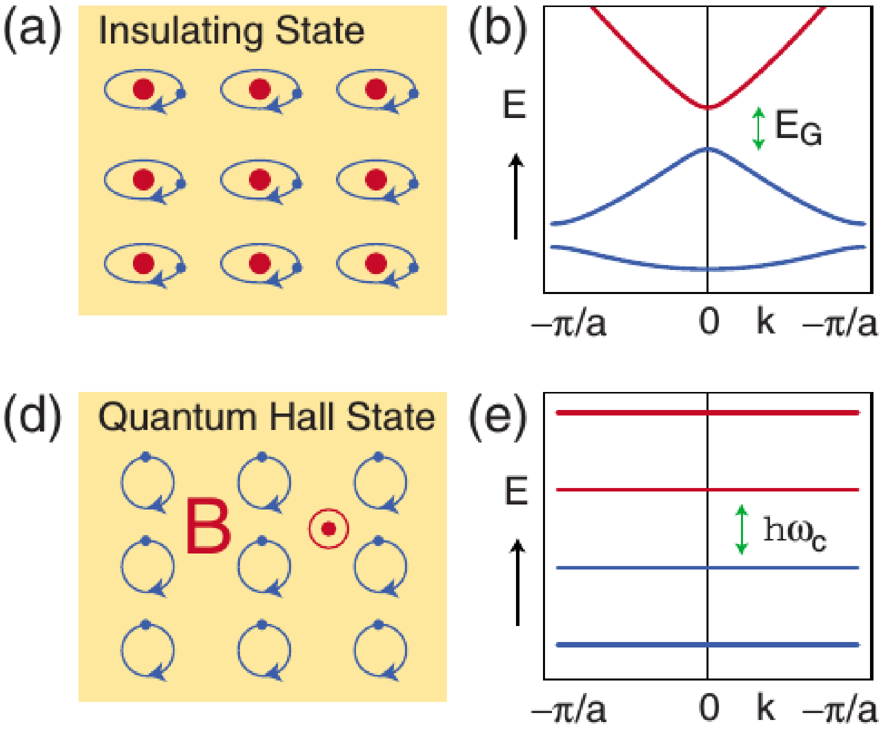
(*a*) The insulating state is characterized by an energy gap separating the occupied and empty electronic states, which is a consequence of the quantization of the energy of atomic orbitals. (*b*) In the quantum Hall effect, the circular motion of electrons in a magnetic field, ***B***, is interrupted by the sample boundary. At the edge, electrons execute “skipping orbits” as shown, ultimately leading to perfect conduction in one direction along the edge. (*c*) The edge of the “quantum spin Hall effect state” or 2D topological insulator contains left-moving and right-moving modes that have opposite spin and are related by time-reversal symmetry. This edge can also be viewed as half of a quantum wire, which would have spin-up and spin-down electrons propagating in both directions. (*d*) The surface of a 3D topological insulator supports electronic motion in any direction along the surface, but the direction of the electron’s motion uniquely determines its spin direction and vice versa. The 2D energy–momentum relation has a “Dirac cone” structure similar to that in graphene.

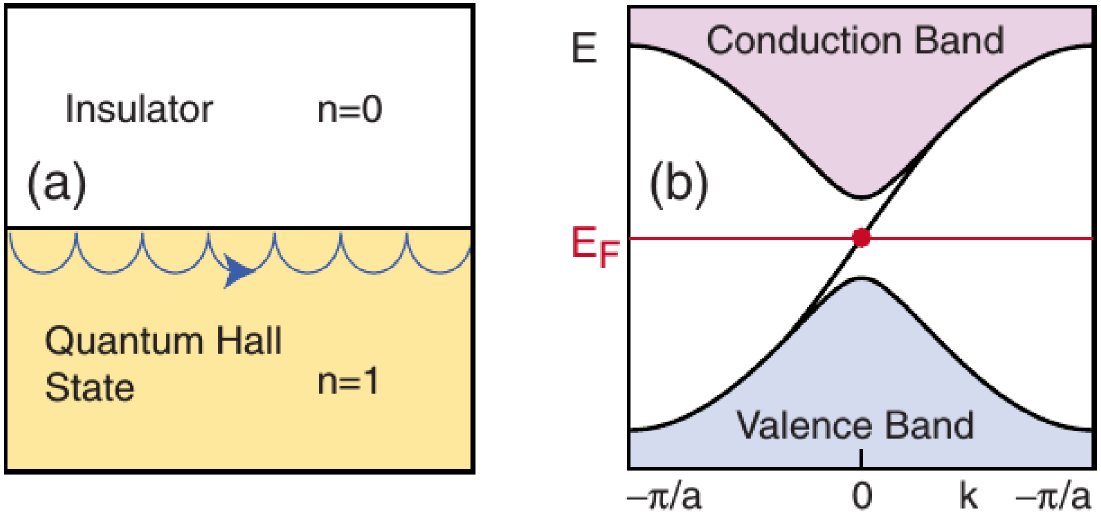
Topologické izolátory

První podobný stav: Kvantový Hallův jev



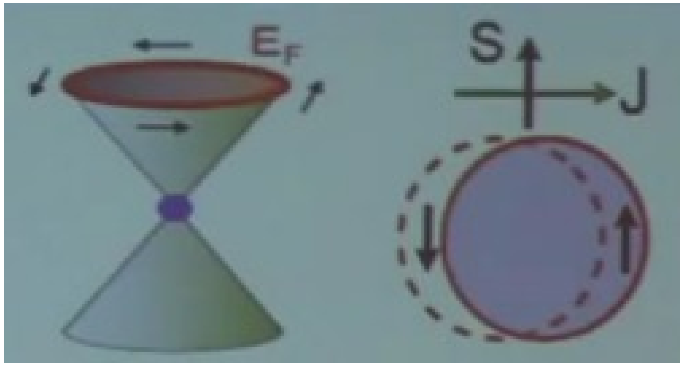






Topologické izolátory

Vlastnosti topologických izolátorů:



- proud je úměrný magnetizaci
  - nové aplikační možnosti
- Absence zpětného rozptylu elektronů
  - vysoké pohyblivosti až 10000cm^2/Vs, elektronika s malým příkonem
- Robustní vůči nemagnetickým nečistotám
  - povrchové stavy jsou důsledkem symetrie

Topologické izolátory

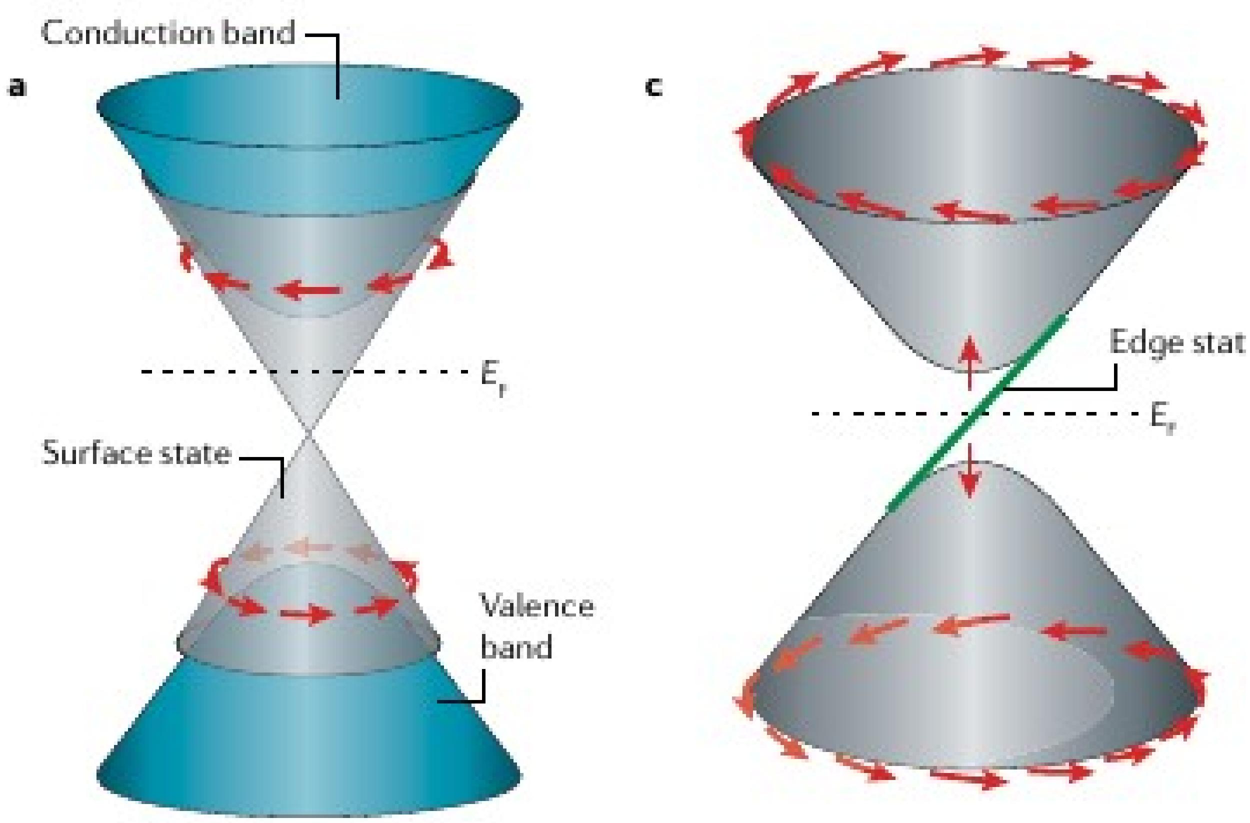
Další možné aplikace:

- kvantové počítače
- spintronické součástky
- ...

Topologický izolátor s feromagnetickým uspořádáním:

- Kvantový anomální Hallův jev

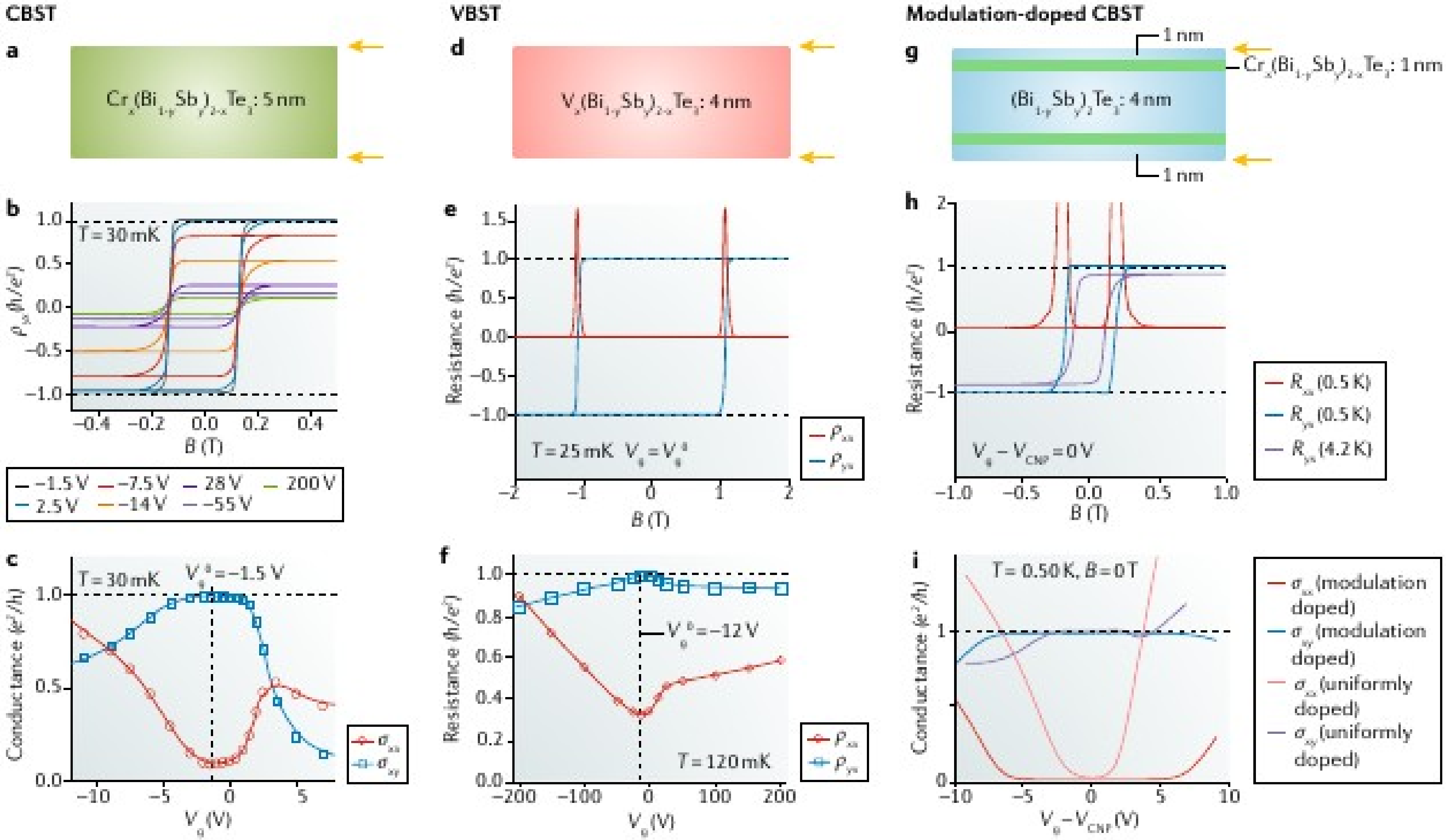
Topologické izolátory



Magnetic topological insulators

Yoshinori Tokura[1,2], Kenji Yasuda[2] and Atsushi Tsukazaki[3]*

Topologické izolátory



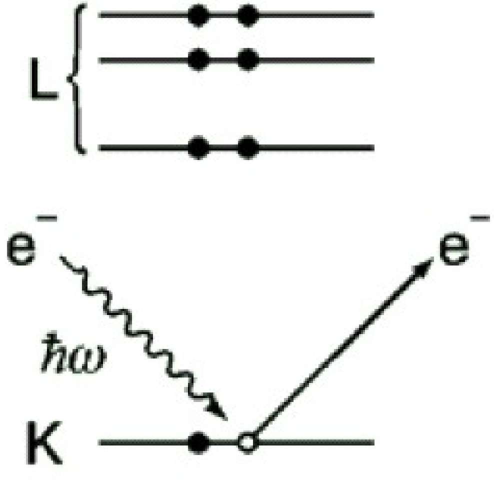
Magnetic topological insulators

Yoshinori Tokura[1,2], Kenji Yasuda[2] and Atsushi Tsukazaki[3]*

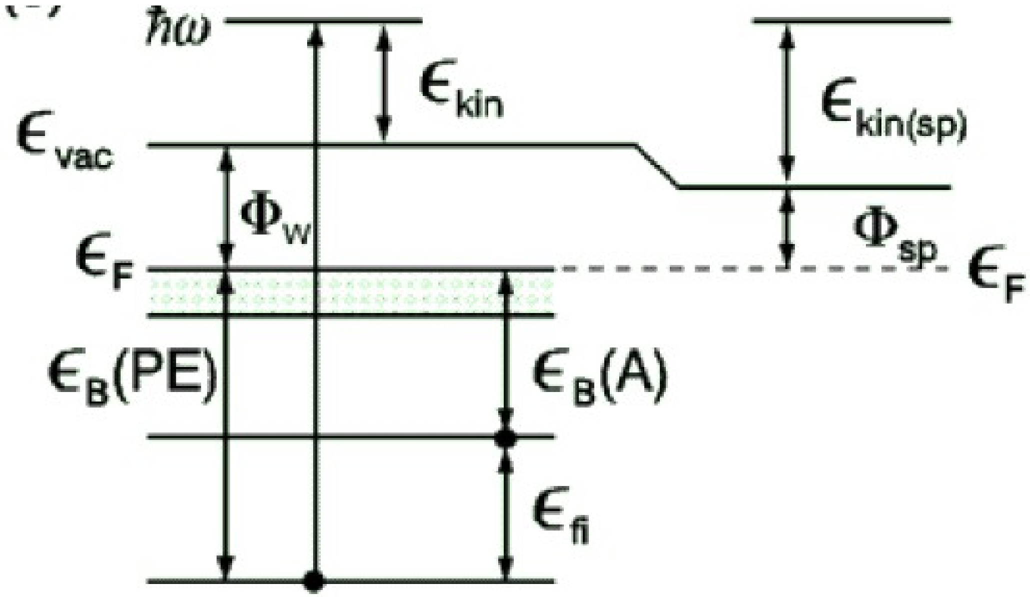
Fotoemise a Augerův jev

Fotoelektrony – přímo vyražené fotonem

Augerovy elektrony – sekundární emise – alternativní proces ke vzniku charakteristického rtg záření.



photoemission



vzorek spektrometr

Fotoelektronová spektroskopie

Podmínky experimentu:

Energie fotonů: 10 až 2000eV

Laboratorní zdroje:

- He výbojka 21 eV
- Mg lampa 1254 eV
- Al lampa 1486 eV

Synchrotron – laditelný zdroj

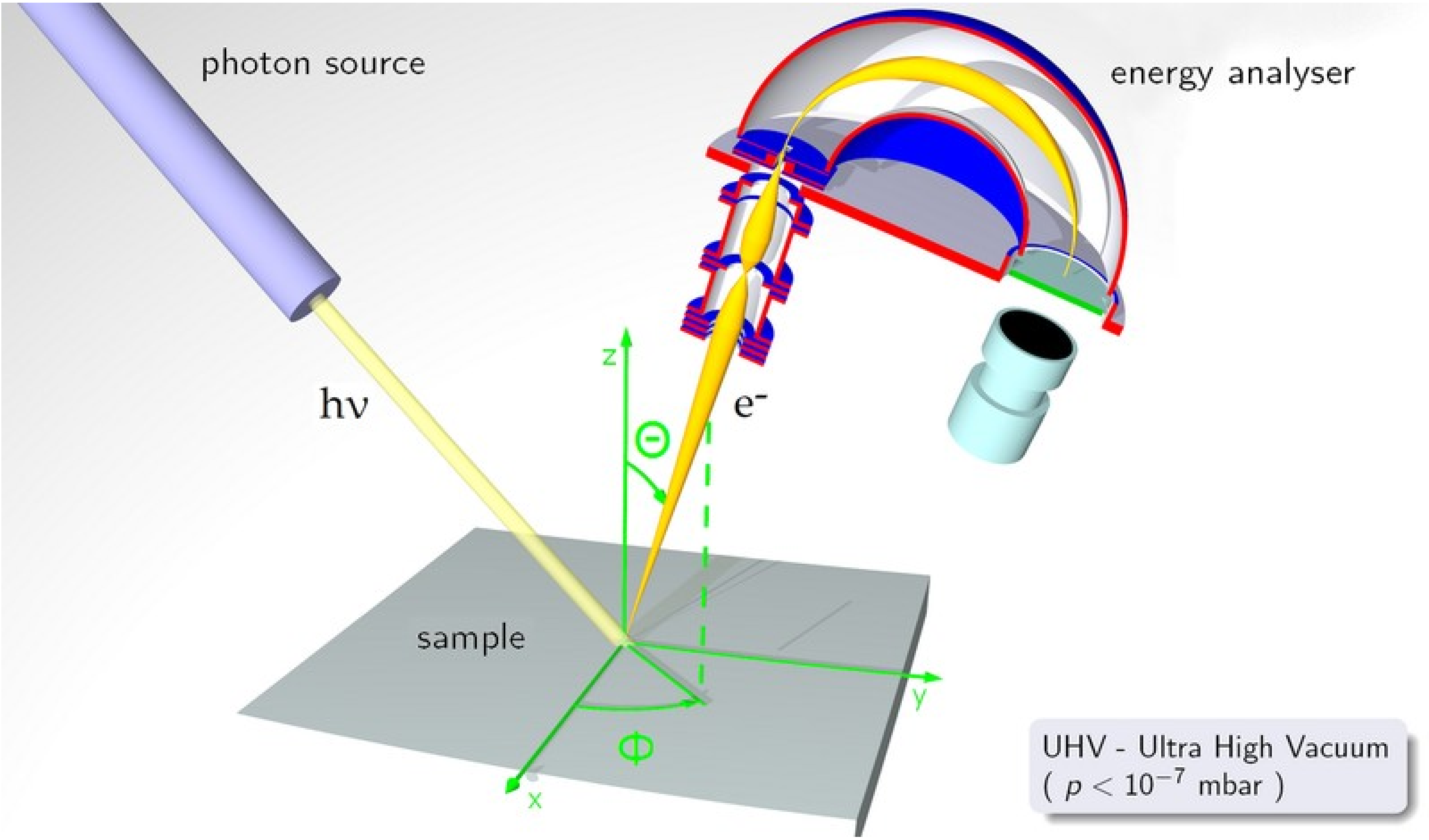
Vysoké vakuum (tlak max 10^{-6} Pa)

Vysoká kvalita a čistota povrchu vzorků

Optika – jen na odraz – zrcadla, difrakční mřížky, žádná okénka!

Hloubka vniku 10^{0} – 10^{1} nm

ARPES - úhlově rozlišená



UHV - Ultra High Vacuum
($p < 10^{-7}$ mbar)

ARPES

Zákony zachování

- Kvaziimpulz – zachovává se tečná složka

$$\hbar\vec{k}_{\mathrm{foton},\|} + \hbar\vec{k}_{i,\|} = \hbar\vec{k}_{f,\|}$$

$$\hbar\vec{k}_{i,\|} \approx \hbar\vec{k}_{f,\|} = \sqrt{2mE}\sin\theta$$

$$\hbar\vec{k}_x = \sqrt{2mE}\sin\theta\cos\phi$$

$$\hbar\vec{k}_y = \sqrt{2mE}\sin\theta\sin\phi$$

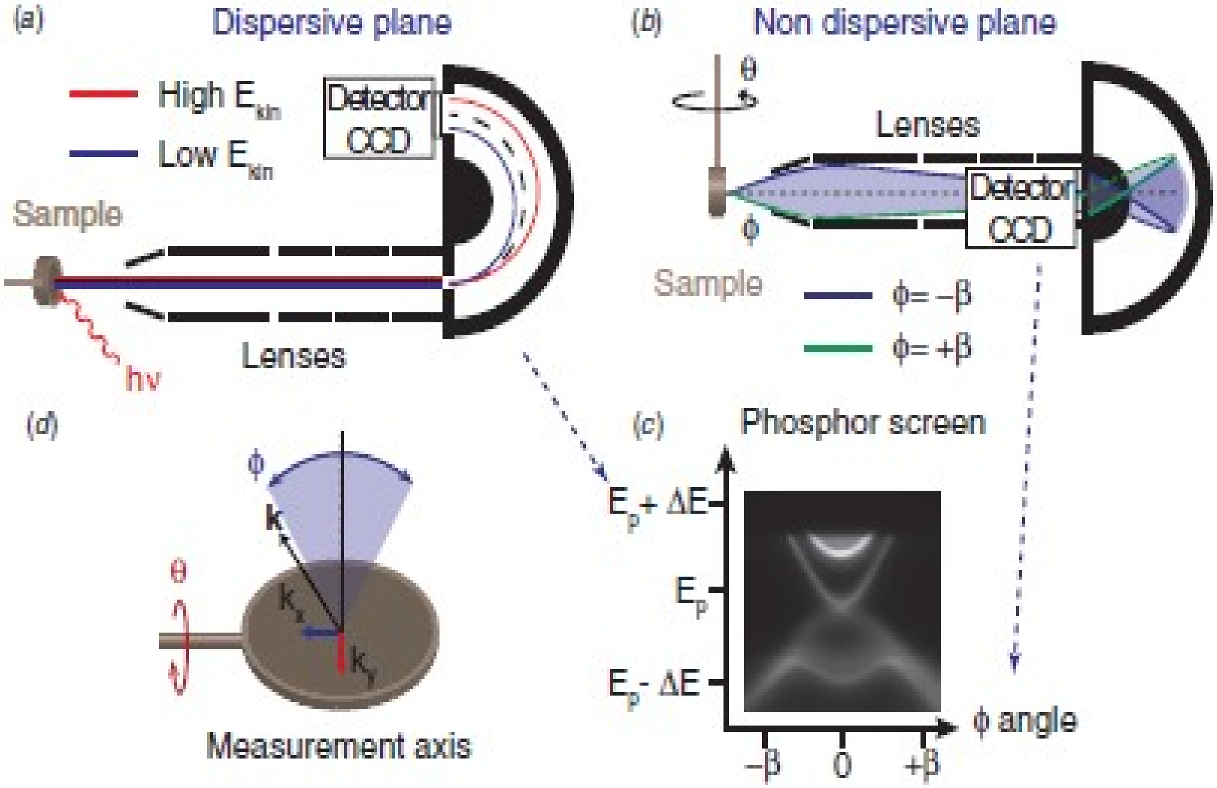
$$\hbar\vec{k}_z = \sqrt{2mE}\cos\theta$$

- energie

$$E_{\mathrm{bound}} = \hbar\omega_i - E_{\mathrm{kin,elektron}} - \varphi$$

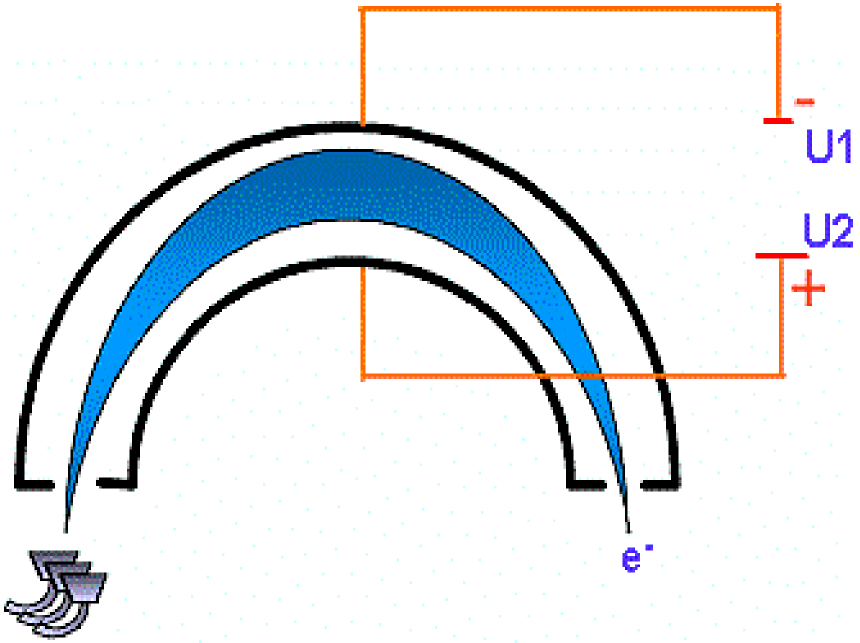
$$\mathbf{k}_{\parallel} = (\sin(\phi)\hat{\mathbf{x}} + \cos(\phi)\sin(\theta)\hat{\mathbf{y}}) \cdot \sqrt{\frac{2m_e E_{\text{kin}}}{\hbar^2}},$$

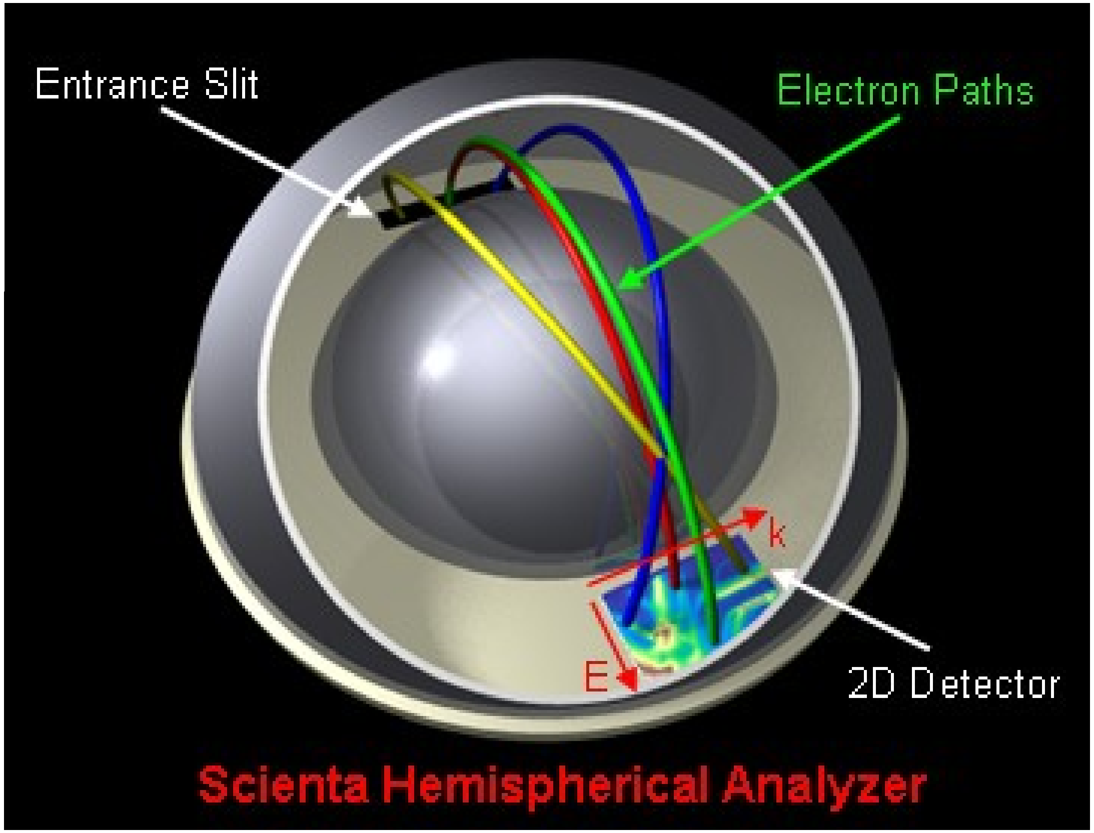
$$k_z = \sqrt{{}^{2m_e}/_{\hbar^2}(V_0 + E_{\text{kin}}\cos(\theta))}.$$



ARPES

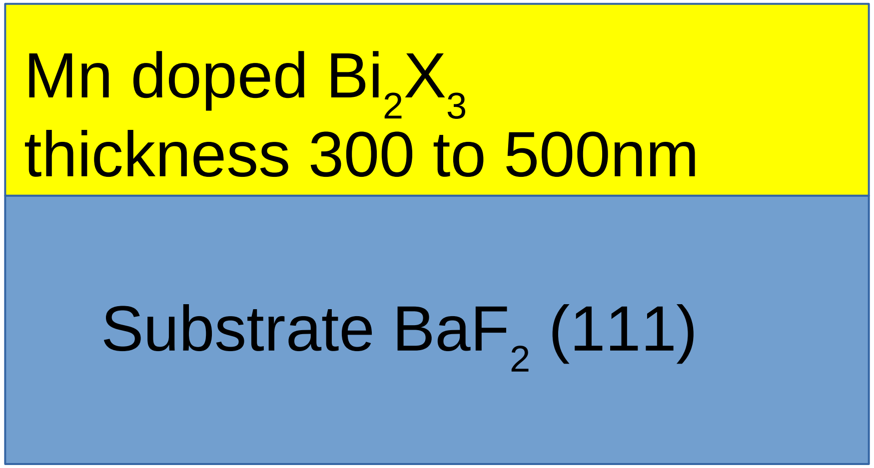
Hemisférický analyzátor + CCD





Sample preparation

G. Springholz group, JKU Linz



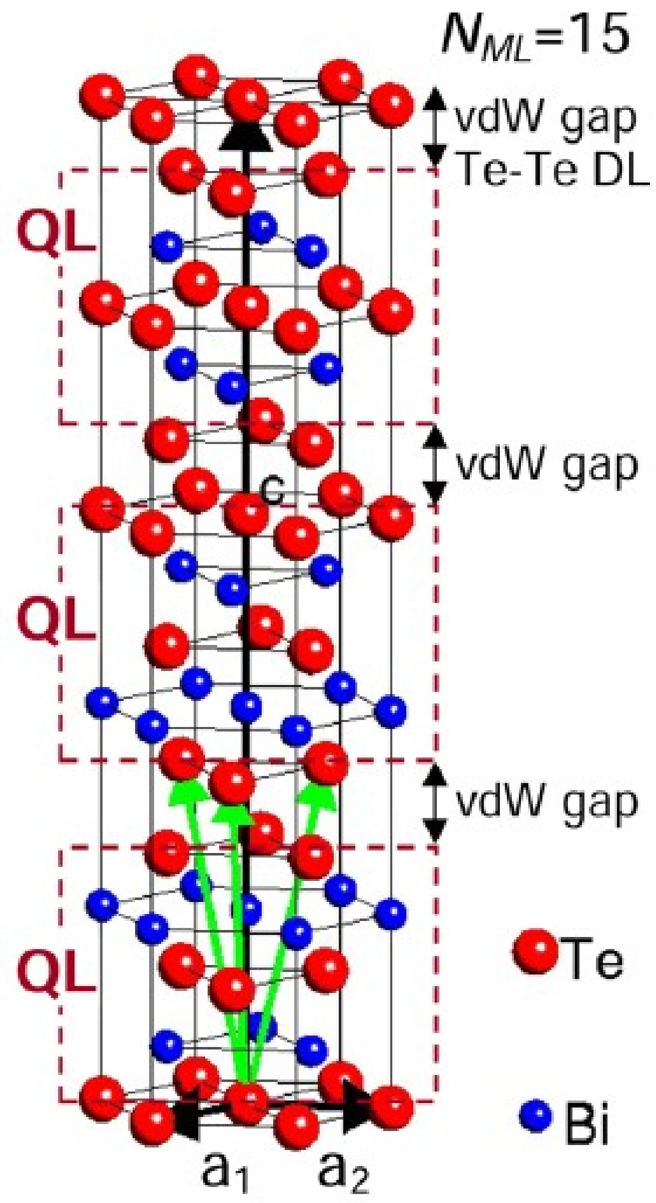
Deposition technique:
Molecular beam epitaxy

Compound sources:
Bi_2Te_3/ Bi_2Se_3, additional Te/Se cell to achieve correct stoichiometry

Sample series:
Bi_2Te_3 up to 11% of Mn doping
Bi_2Se_3 up to 10% of Mn doping

Topologické izolátory dopované Mn

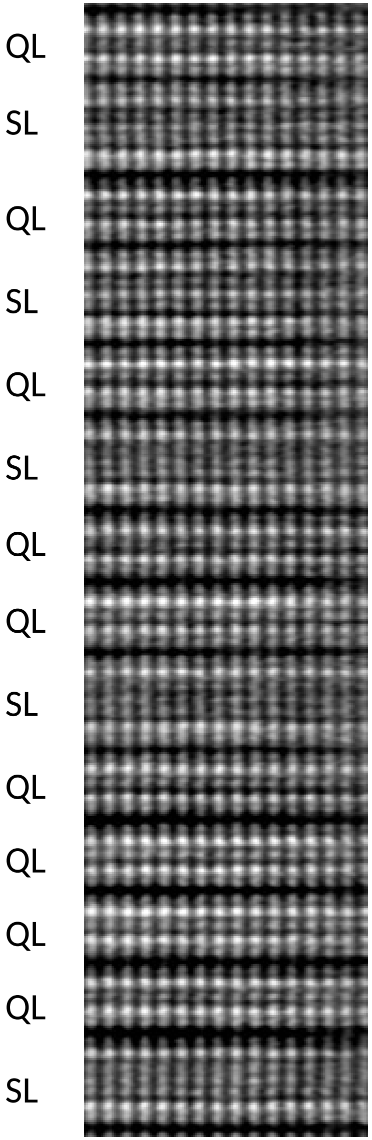
Strukturní analýza vrstev topologických izolátorů



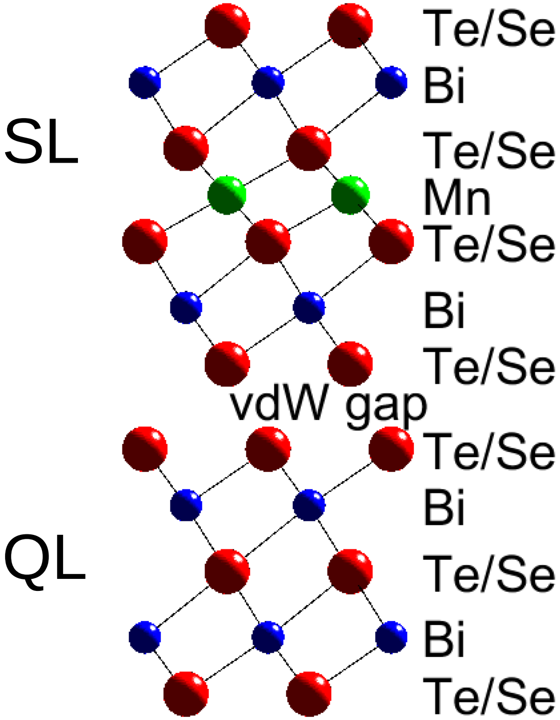
Electron microscopy

JKU Linz, Graz

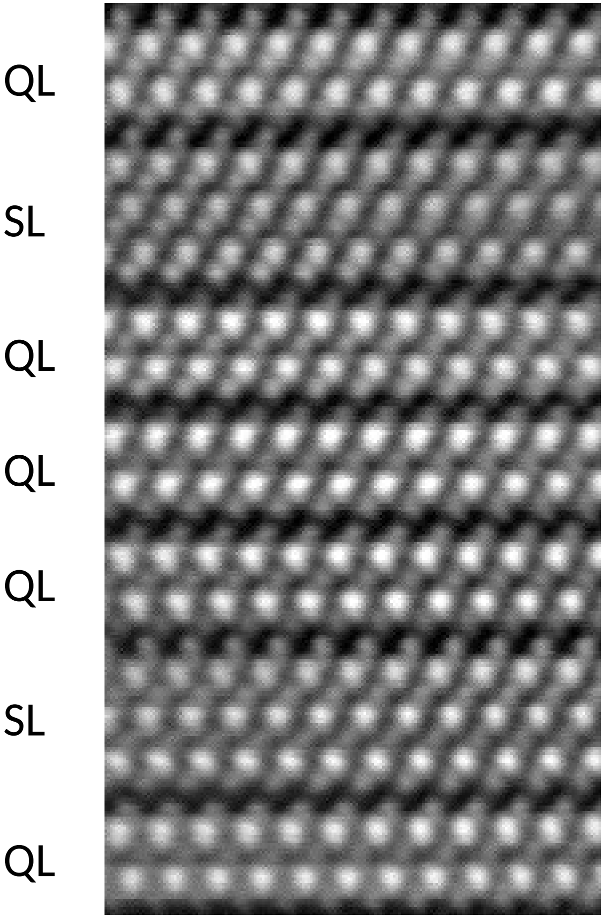
10% Mn Bi_2Te_3



HAADF STEM



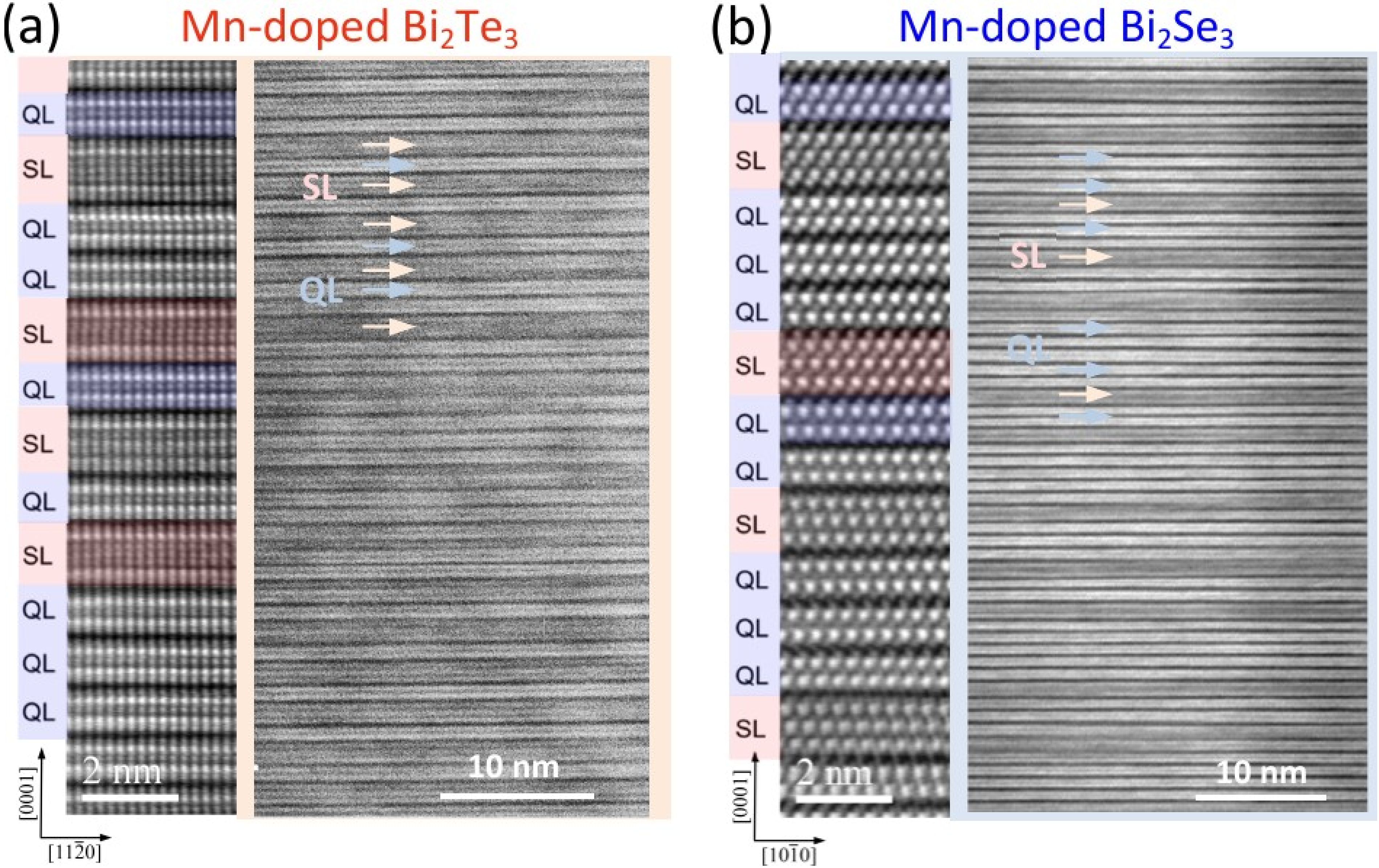
6% $MnBi_2Se_3$



Topologické izolátory dopované Mn

Strukturní analýza vrstev topologických izolátorů

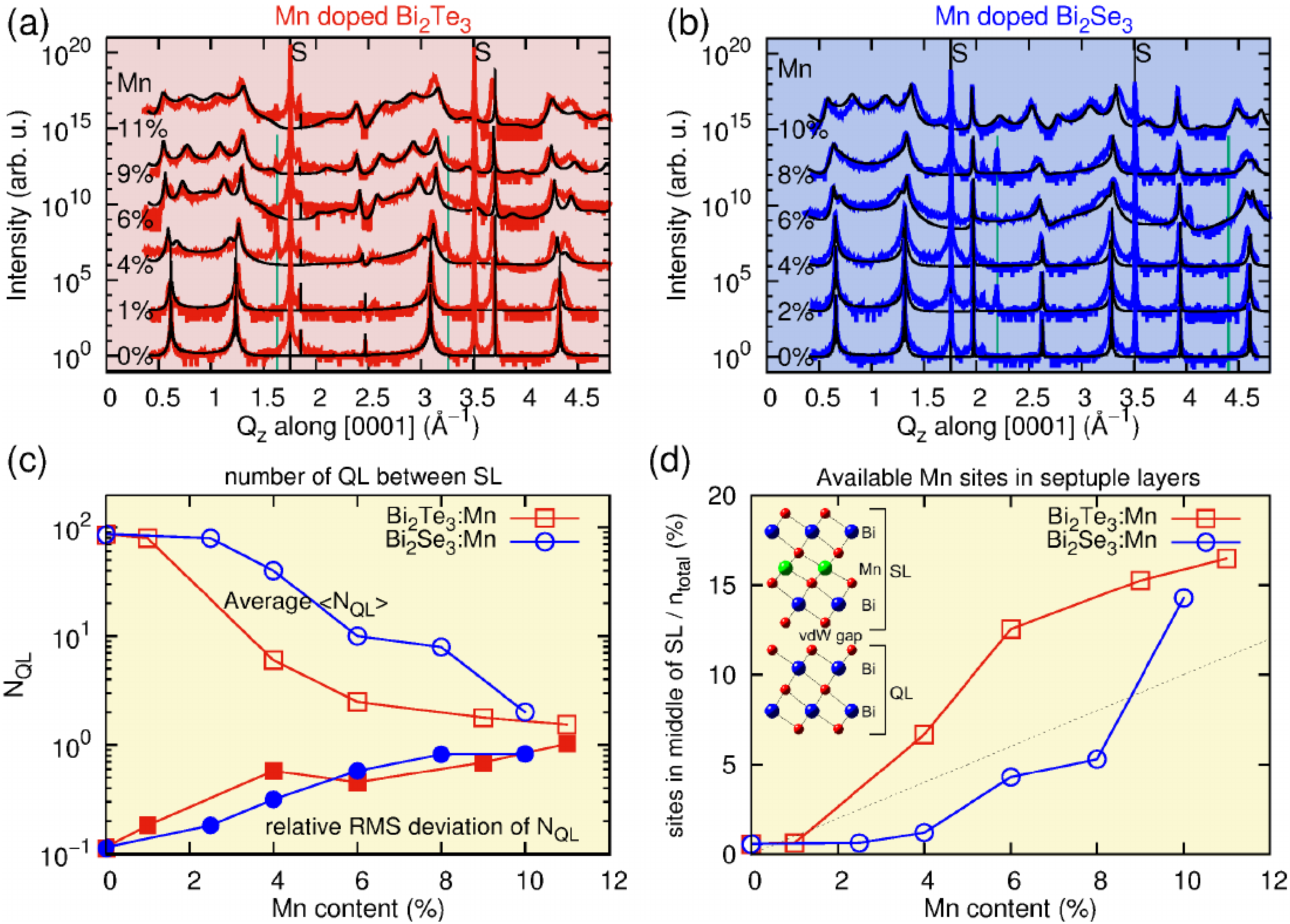
HAADF-STEM (příprava lamel ZONA JKU Linz, TEM Graz)



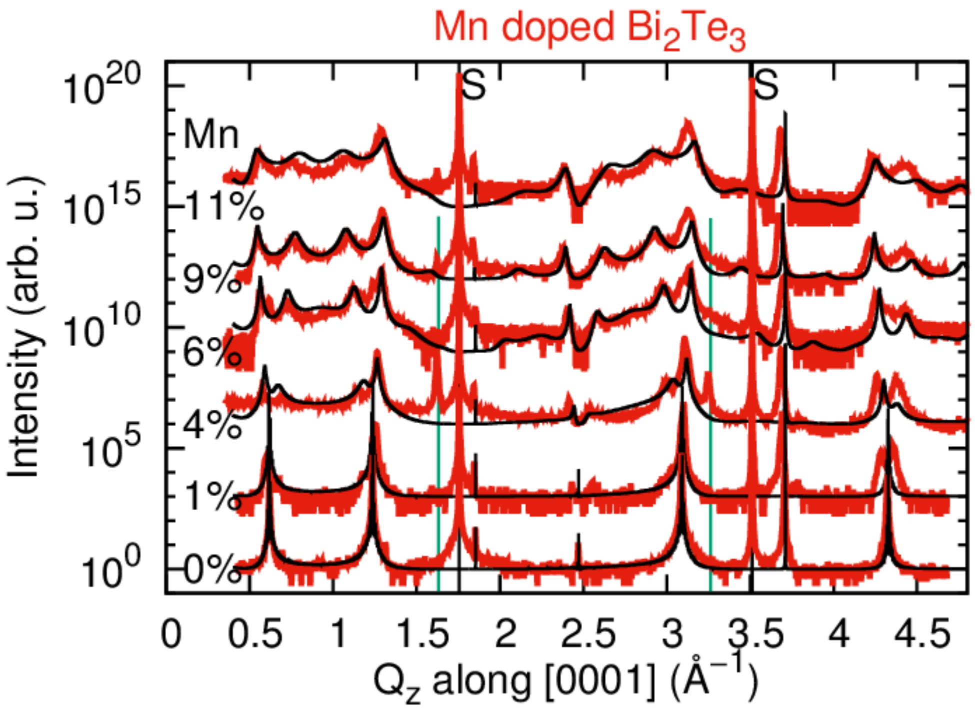
Topologické izolátory dopované Mn

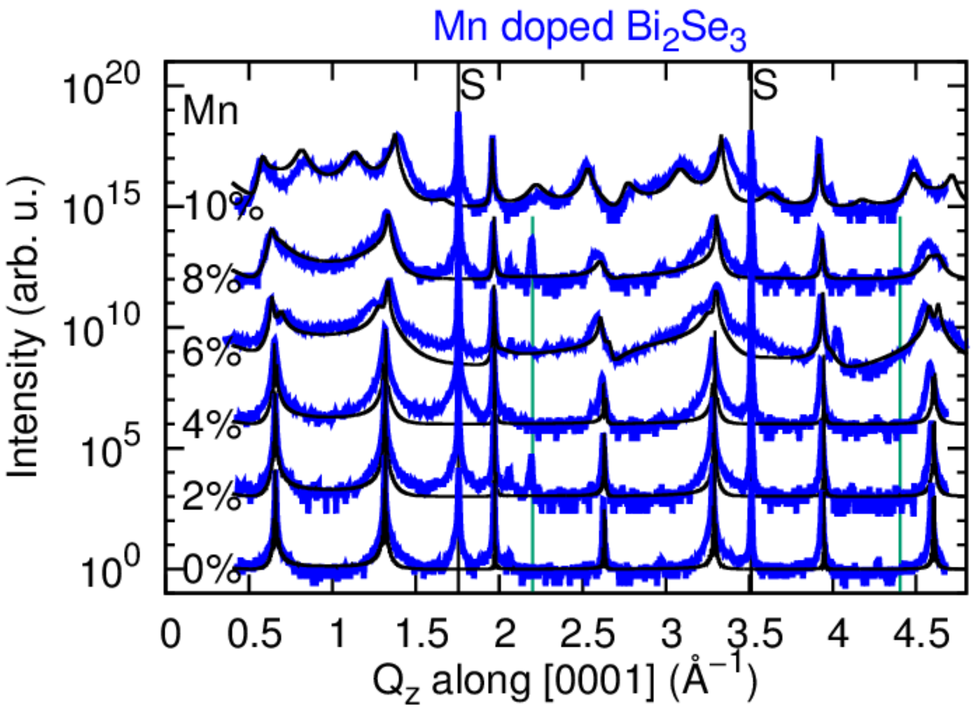
Strukturní analýza vrstev topologických izolátorů

fitováno modelem parakrystalu



XRD structure analysis



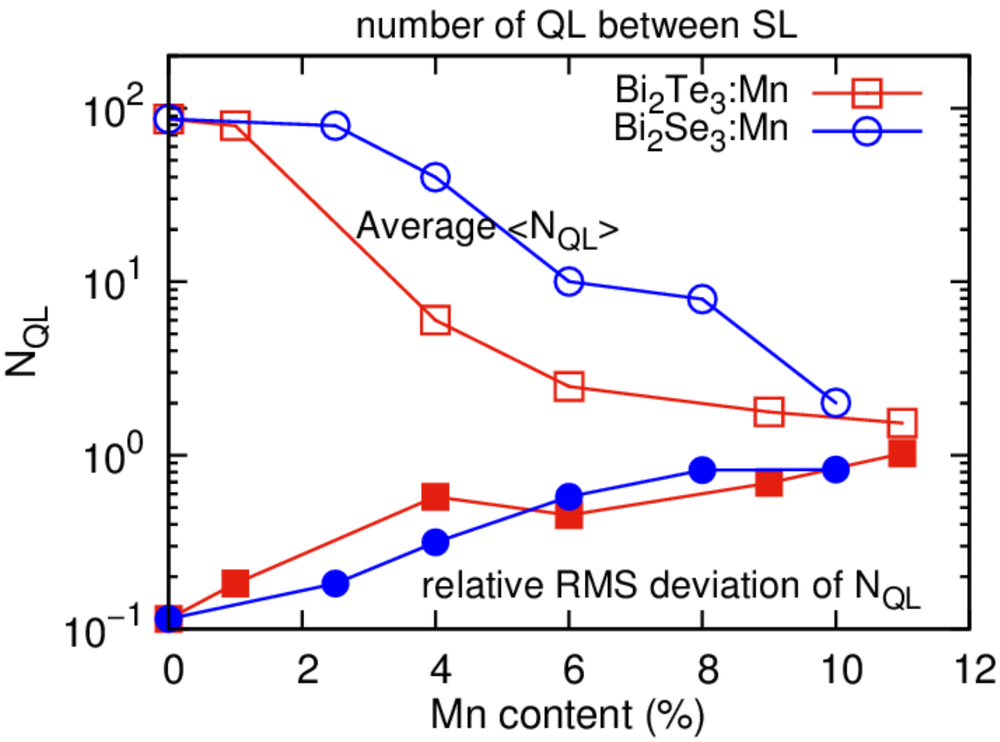


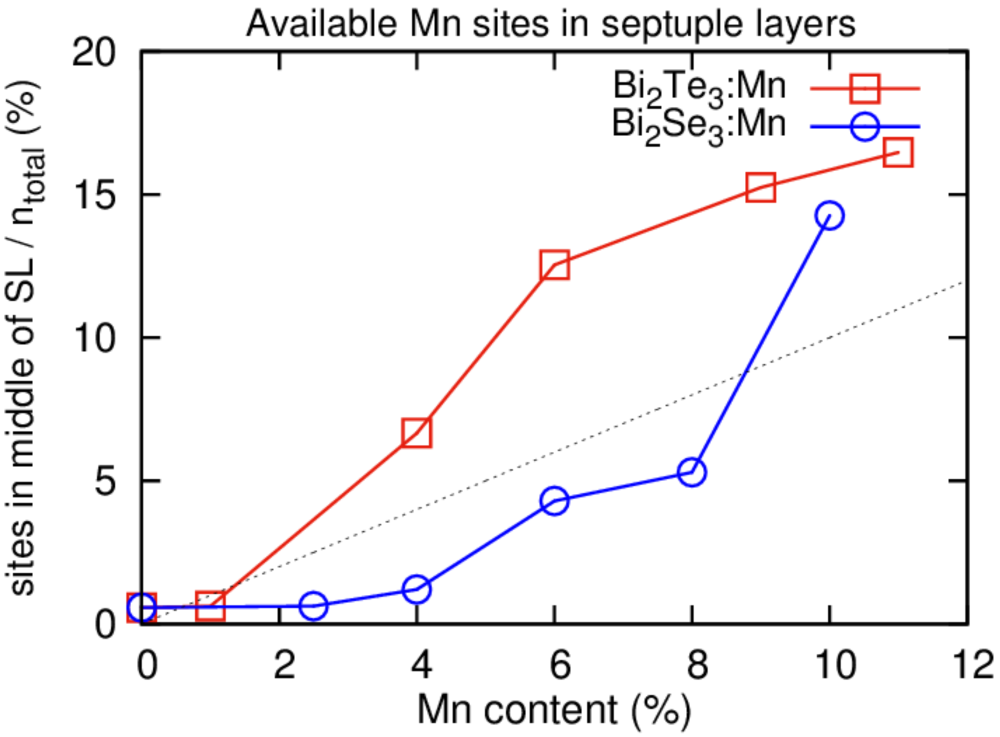
Symmetric scan with scattering vector perpendicular to the surface

Higher Mn content leads to disturbed structure

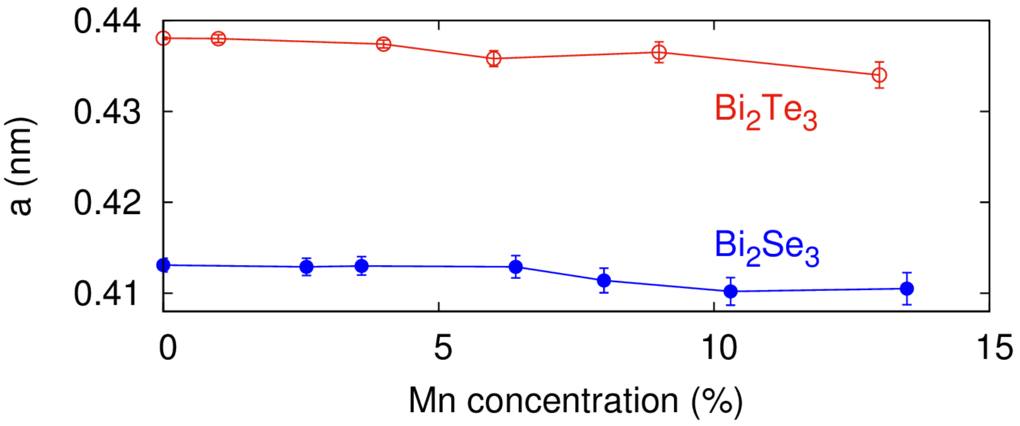
Fitted with a paracrystal model:
Random sequence of Bi_2X_3 (quintuple layers – QL) and
Bi_2MnX_4 (septuple layer – SL)

XRD structure analysis





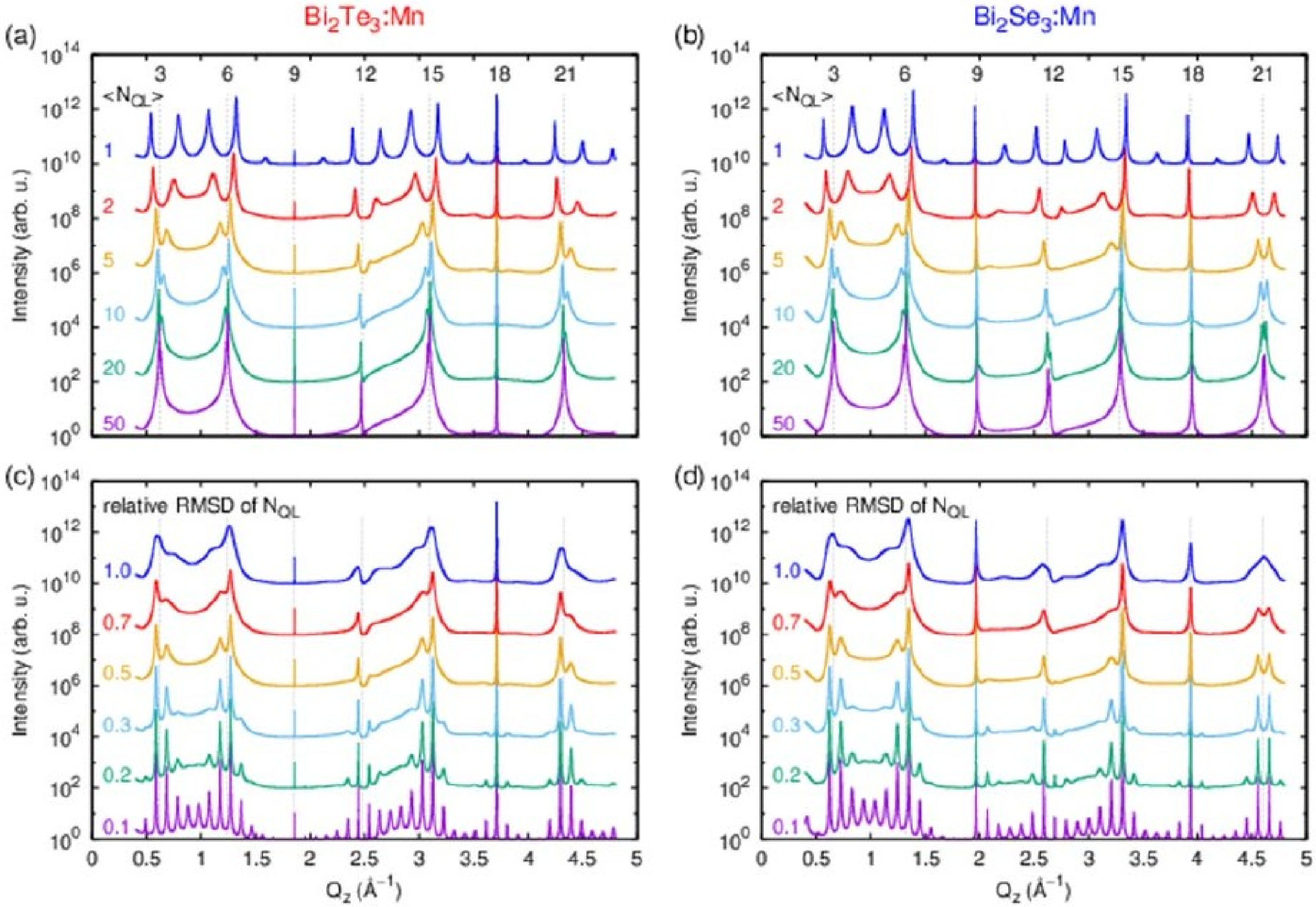
In-plane lattice parameter dependence



Topologické izolátory dopované Mn

Strukturní analýza vrstev topologických izolátorů

fitováno modelem parakrystalu

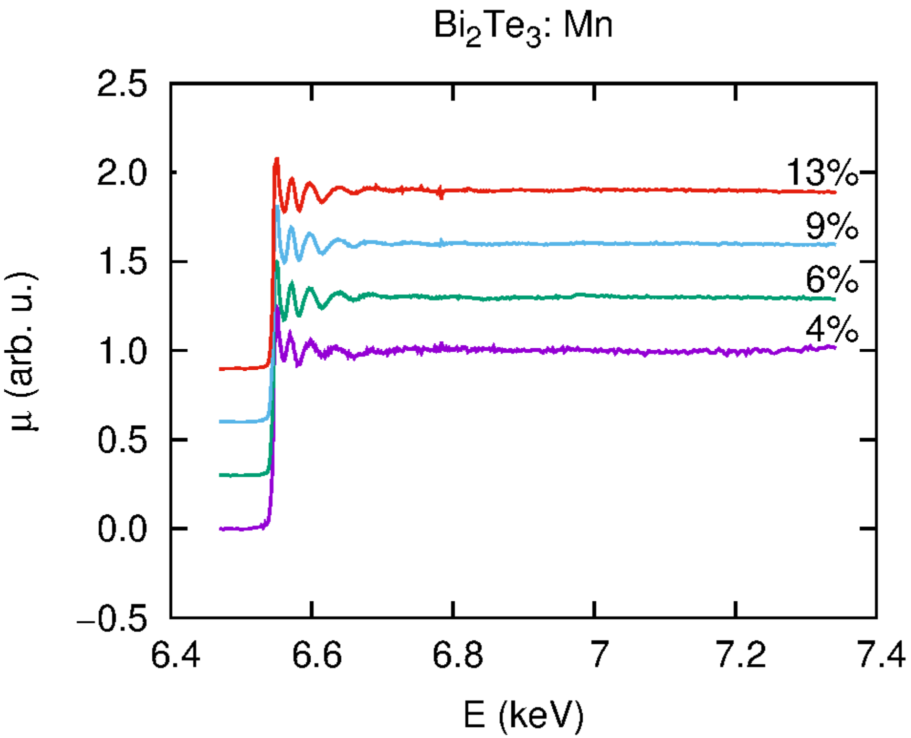


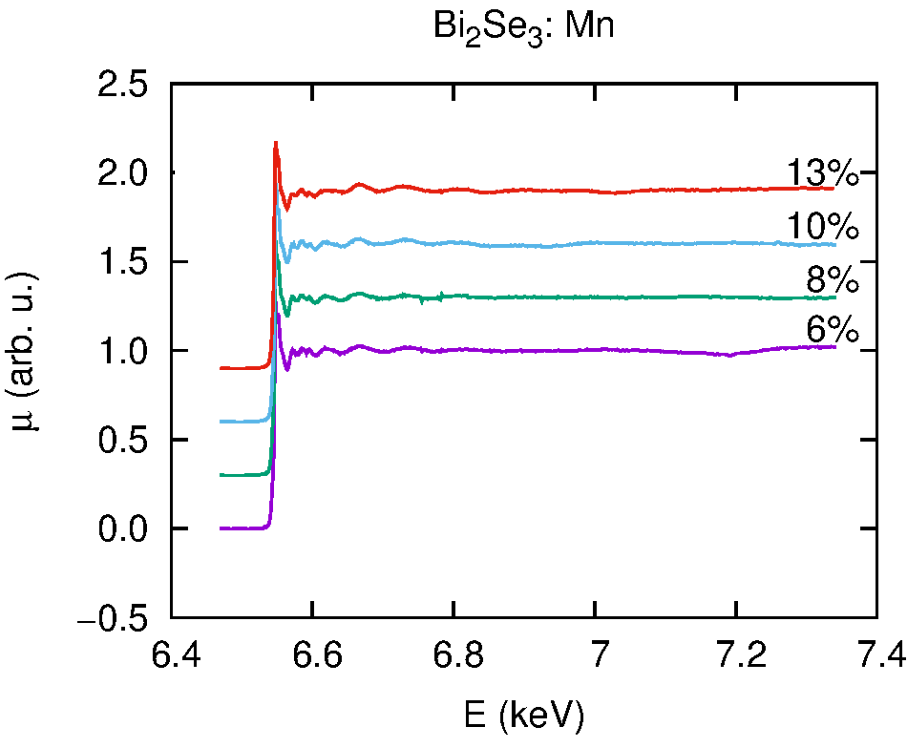
relative
RMSD =0.5

$\langle N_{QL} \rangle$=5

X-ray absorption spectroscopy

Experiment at BM23, ESRF Grenoble

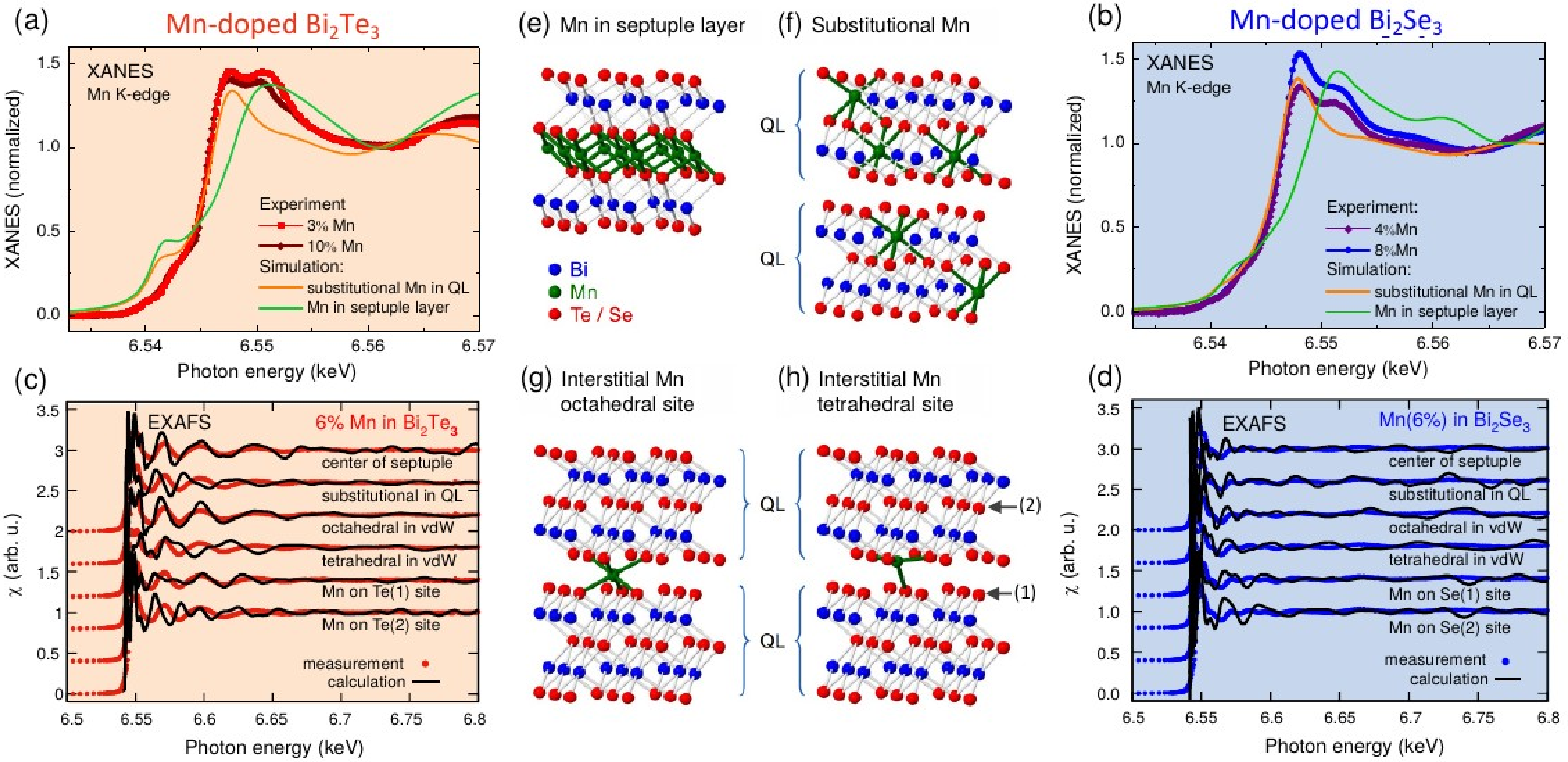

Bi_2Te_3: Mn


Bi_2Se_3: Mn

Very weak Mn concentration dependence

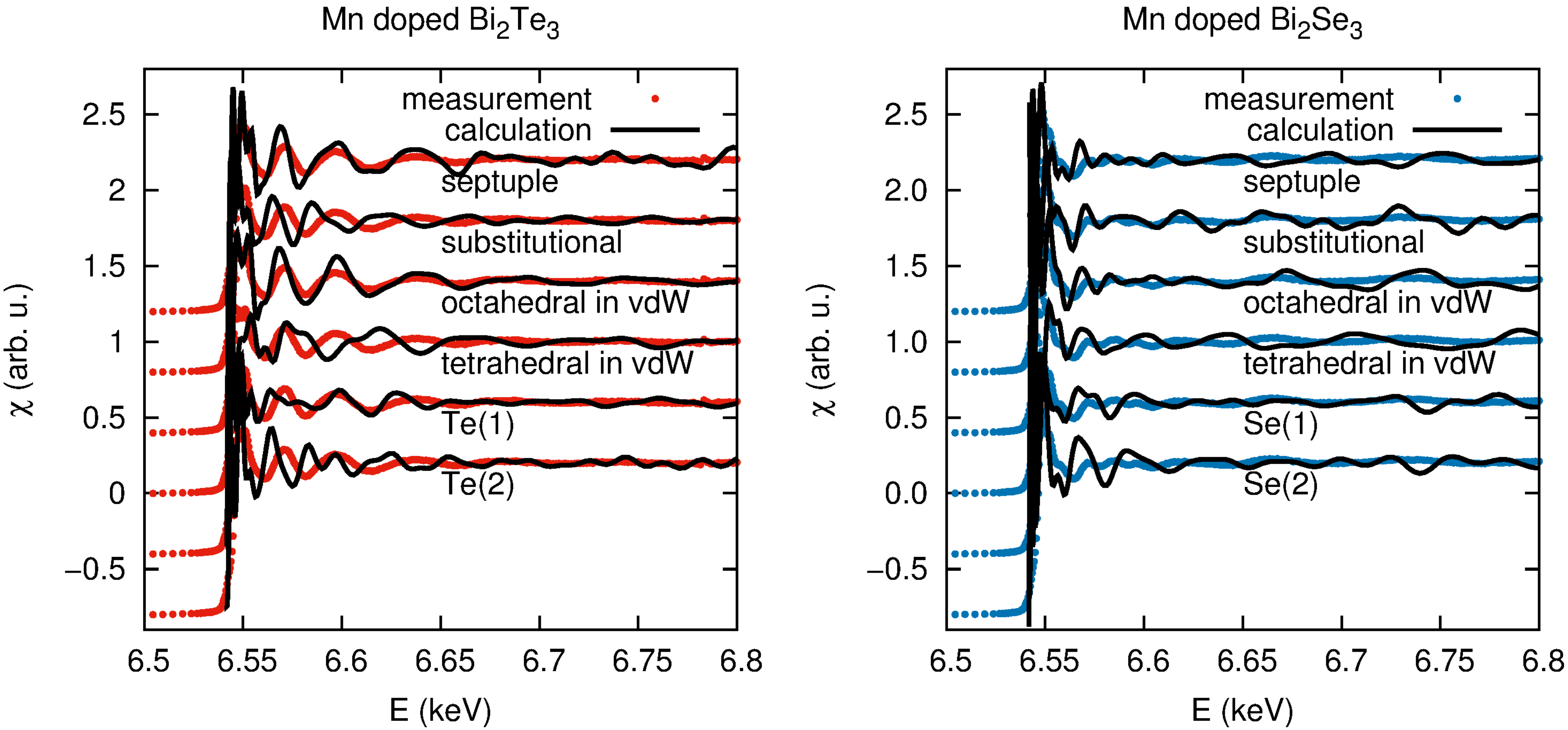
Topologické izolátory dopované Mn

Strukturní analýza vrstev topologických izolátorů



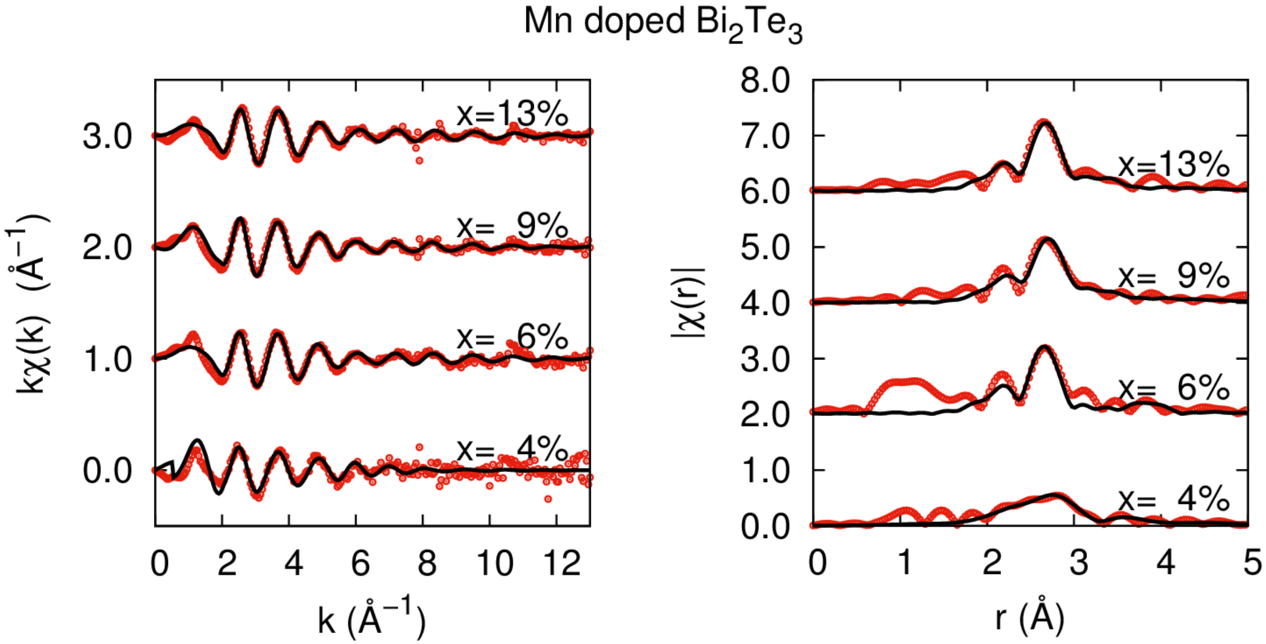
X-ray absorption spectroscopy

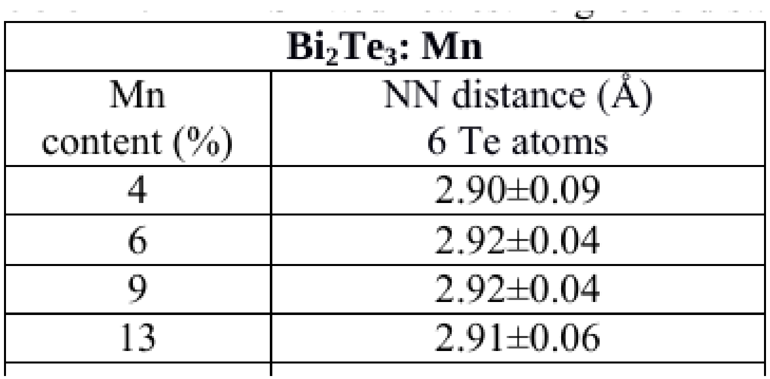
Simulations of various Mn positions



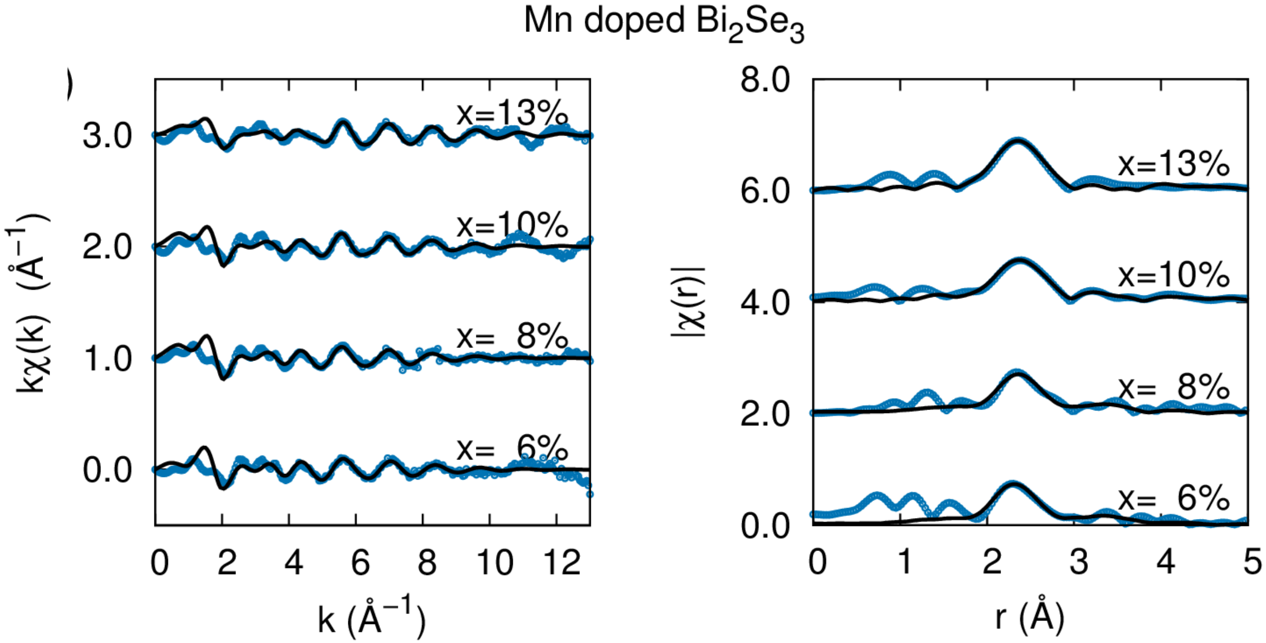
X-ray absorption spectroscopy

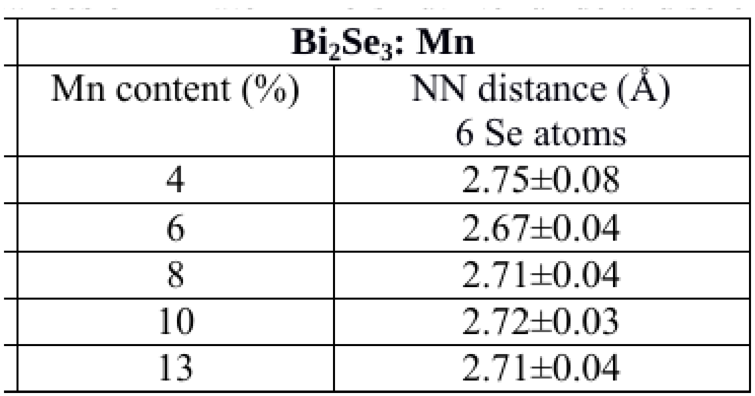
Fitted distances of Mn nearest neighbors


Mn doped Bi_2Te_3



Bi_2Te_3: Mn	
Mn content (%)	NN distance (Å) 6 Te atoms
4	2.90±0.09
6	2.92±0.04
9	2.92±0.04
13	2.91±0.06

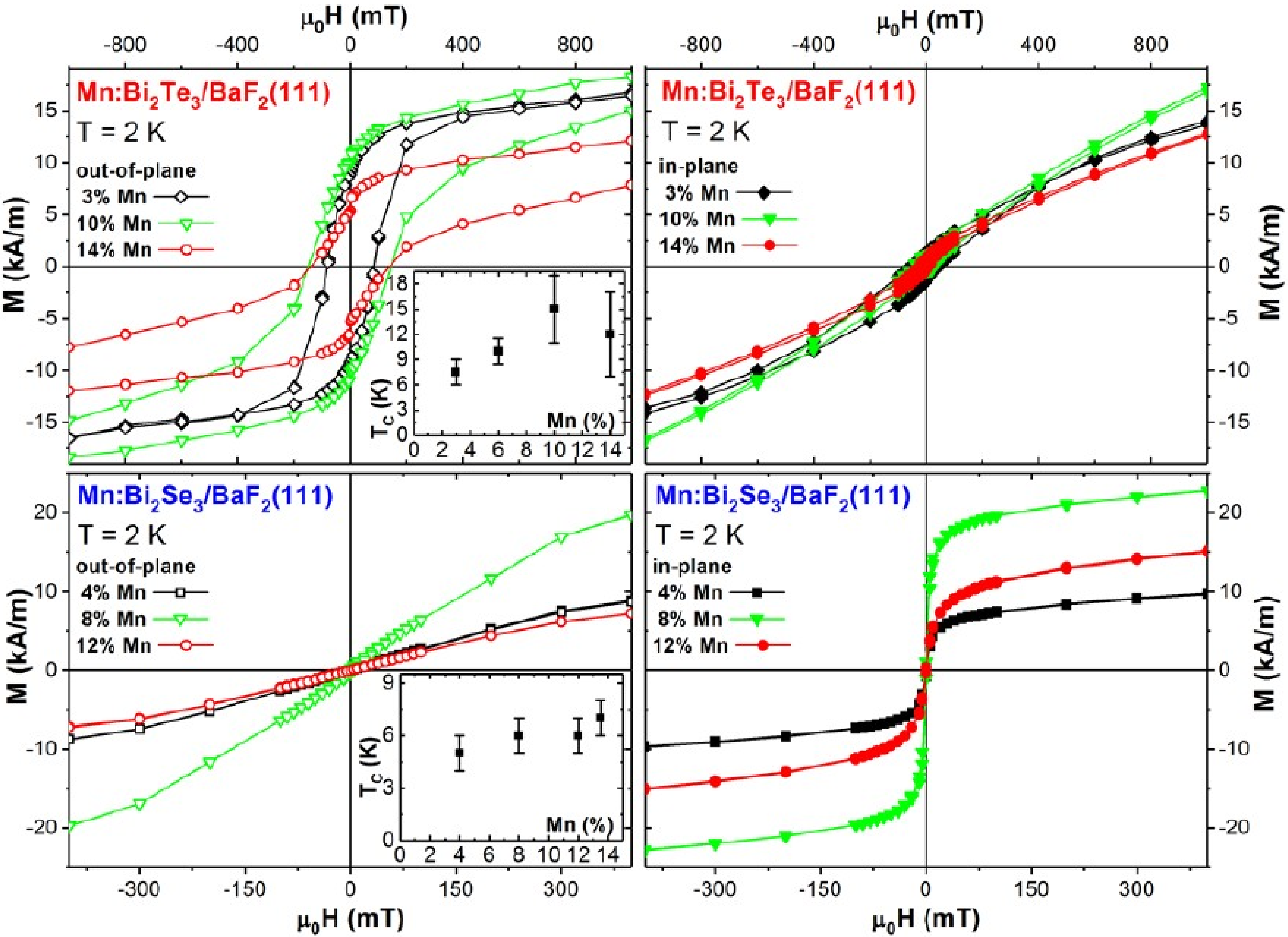

Mn doped Bi_2Se_3



Bi_2Se_3: Mn	
Mn content (%)	NN distance (Å) 6 Se atoms
4	2.75±0.08
6	2.67±0.04
8	2.71±0.04
10	2.72±0.03
13	2.71±0.04

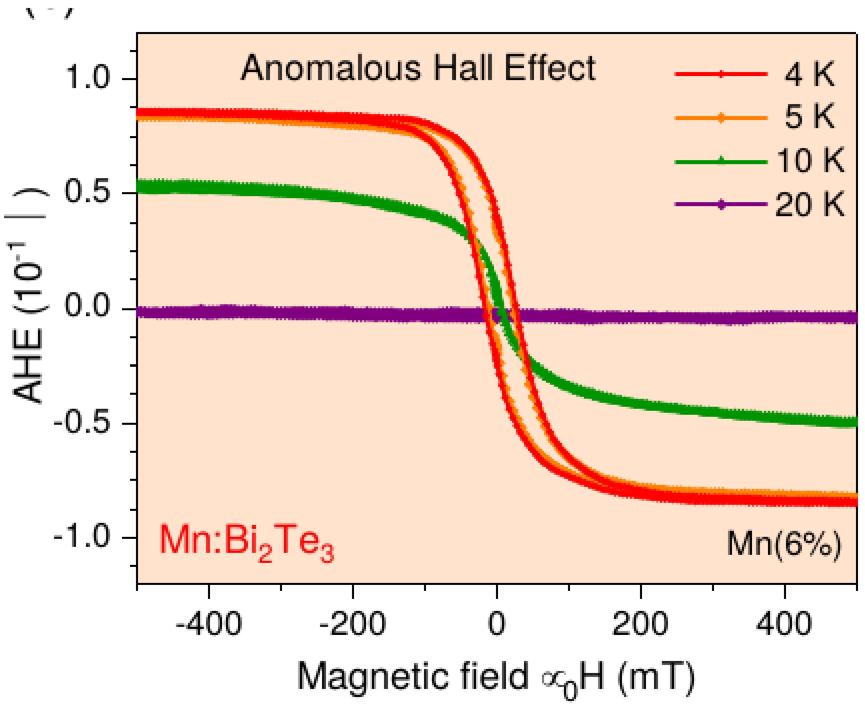
Topologické izolátory dopované Mn

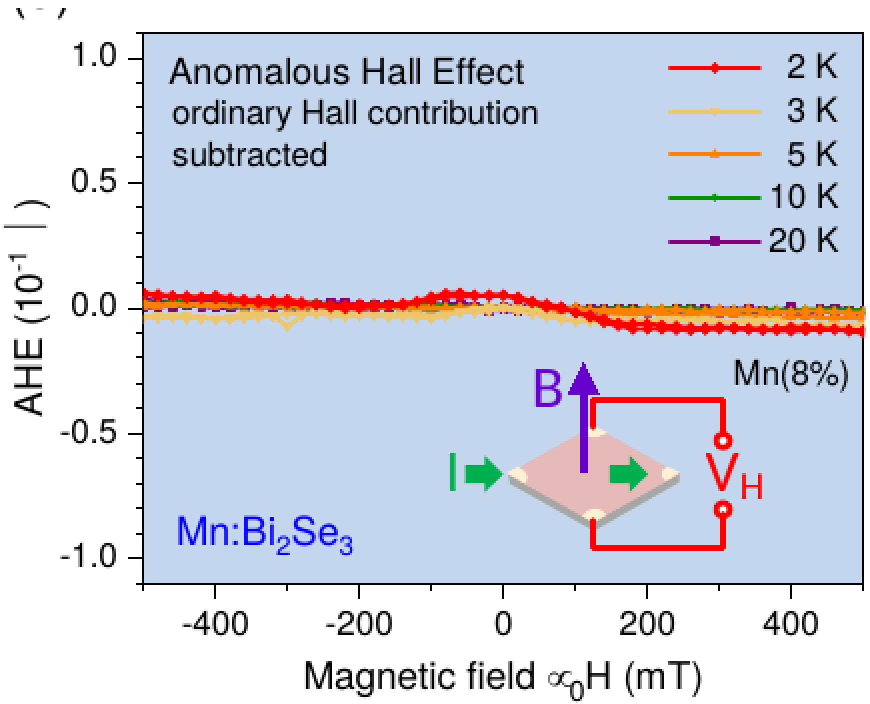
Magnetické vlastnosti vrstev topologických izolátorů
SQUID (JKU Linz)



Topologické izolátory dopované Mn

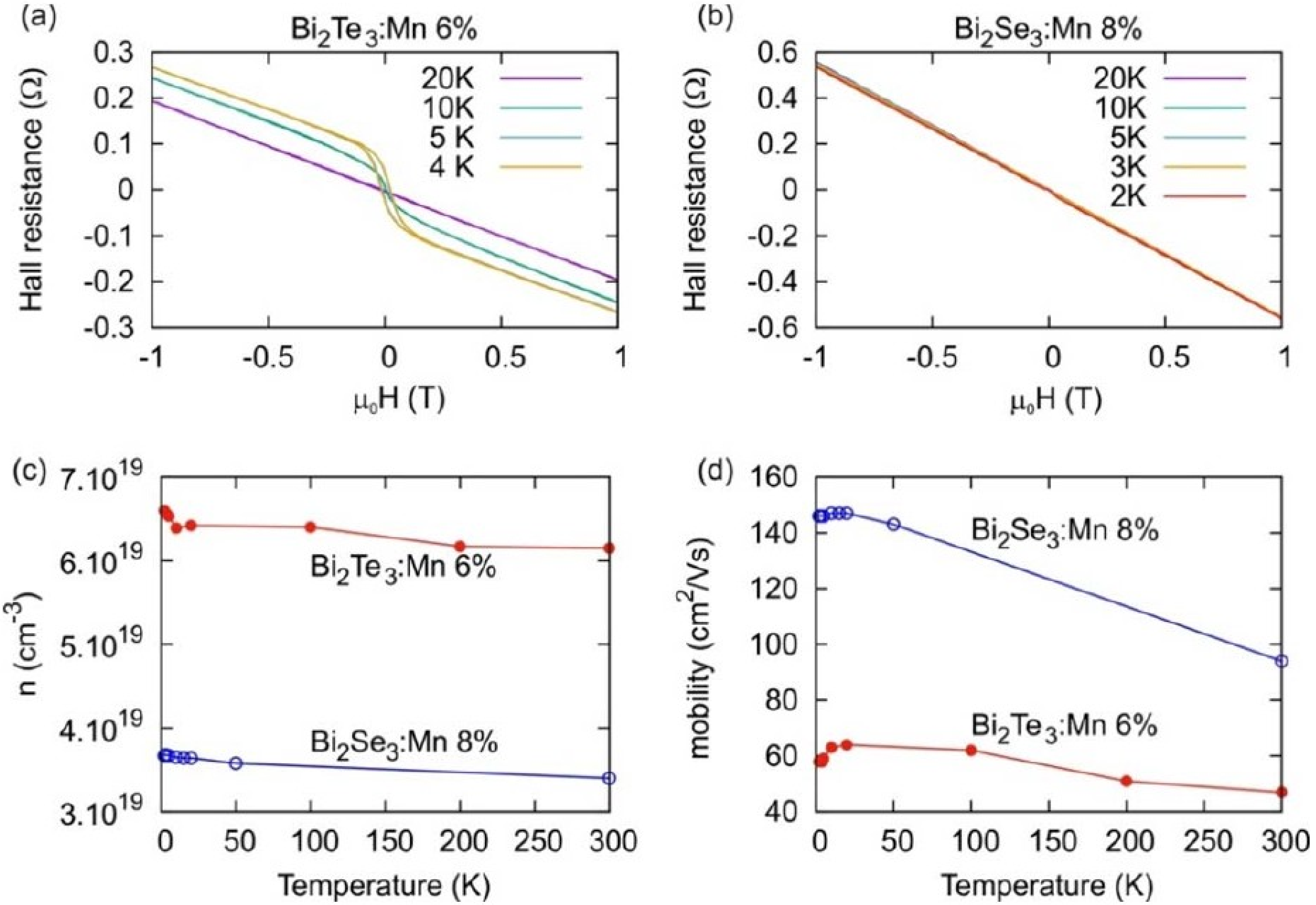
Magnetické vlastnosti vrstev topologických izolátorů - CEITEC





Topologické izolátory dopované Mn

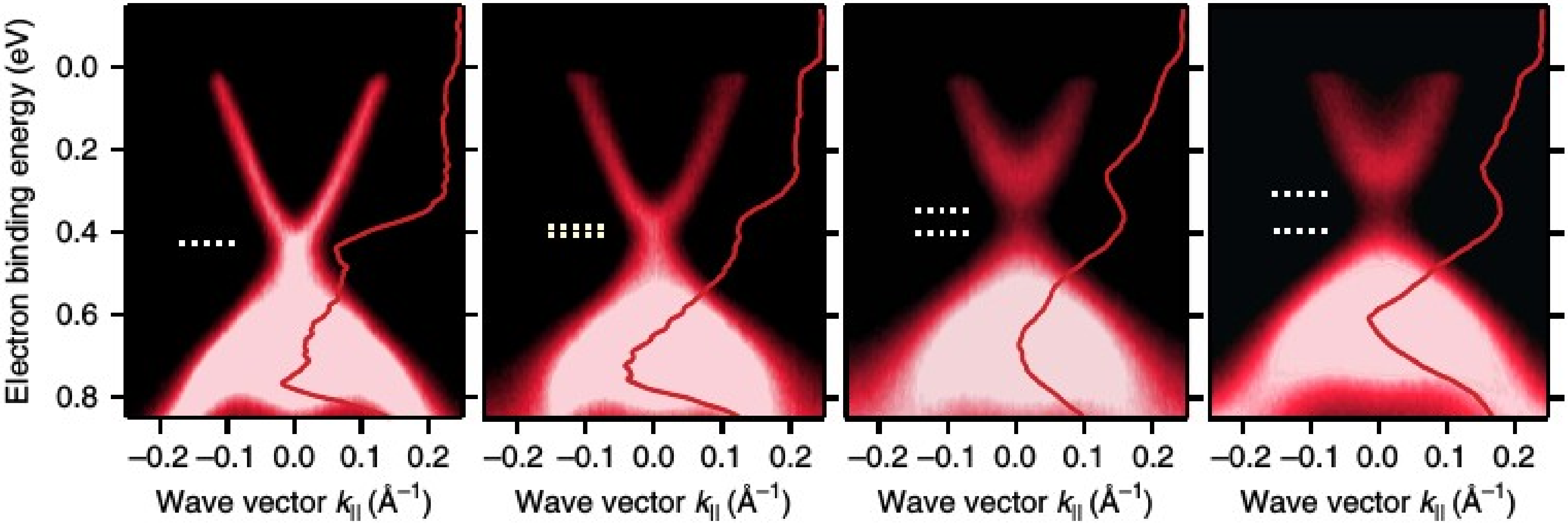
Magnetické vlastnosti vrstev topologických izolátorů - CEITEC



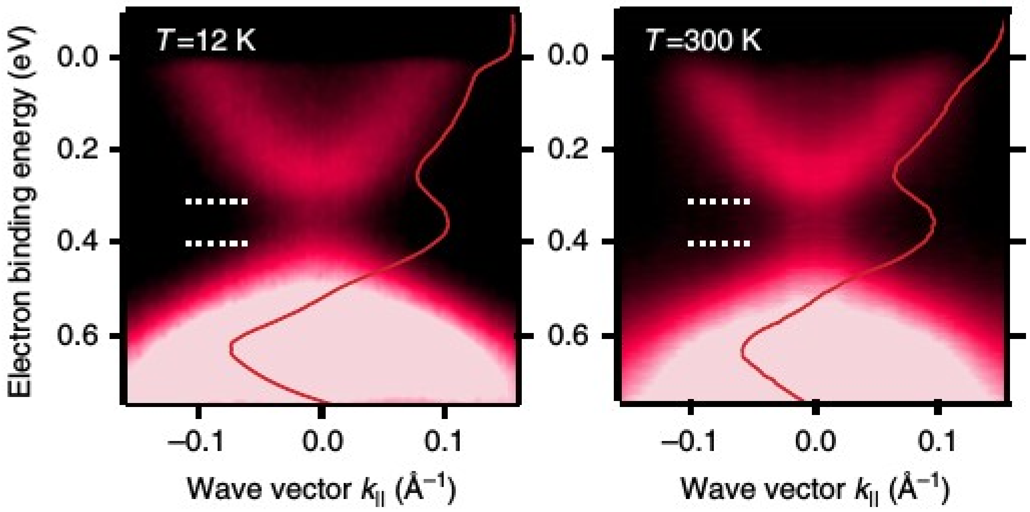
Electronic structure

ARPES BESSYII, HZB Berlin Bi_2Se_3, 12K

Mn 0% 2% 4% 8%



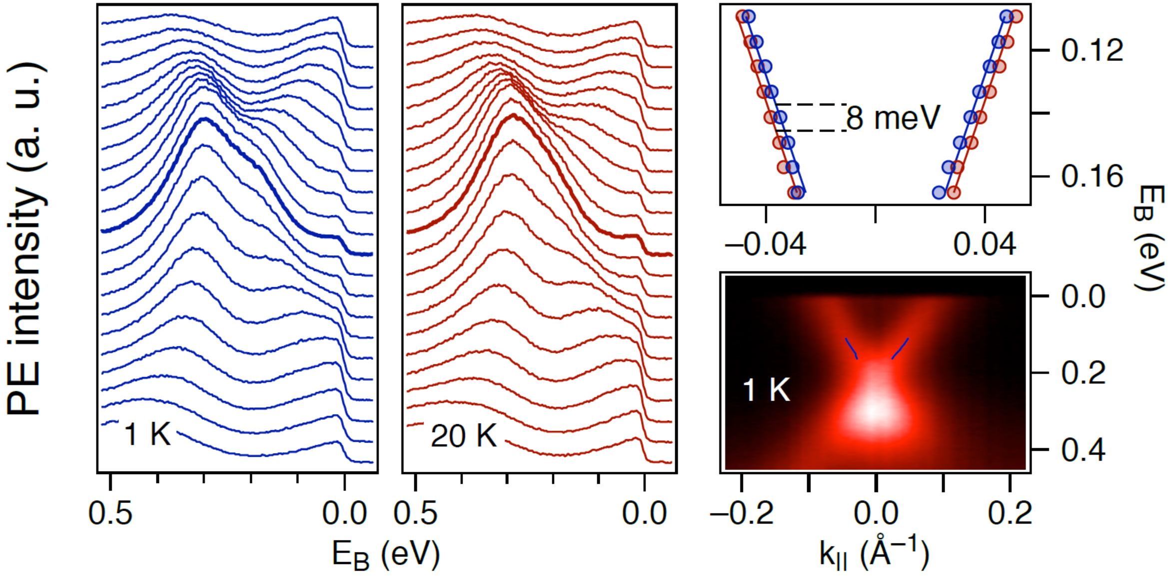
Mn 8%

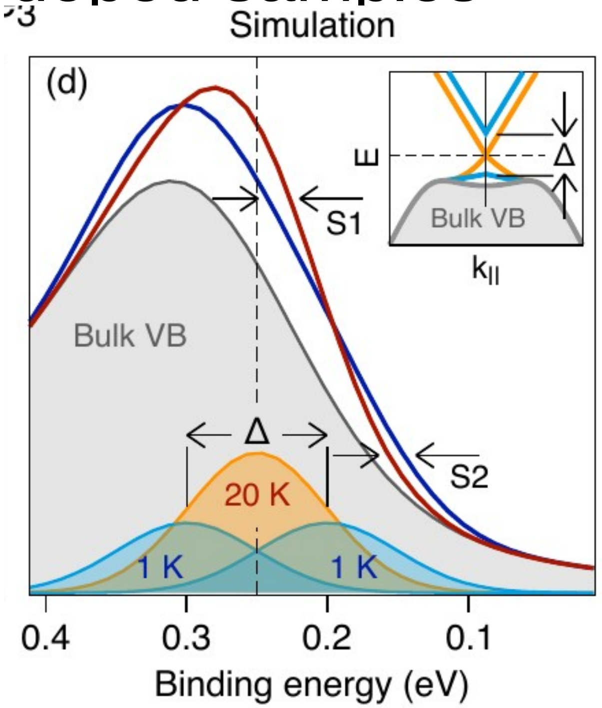


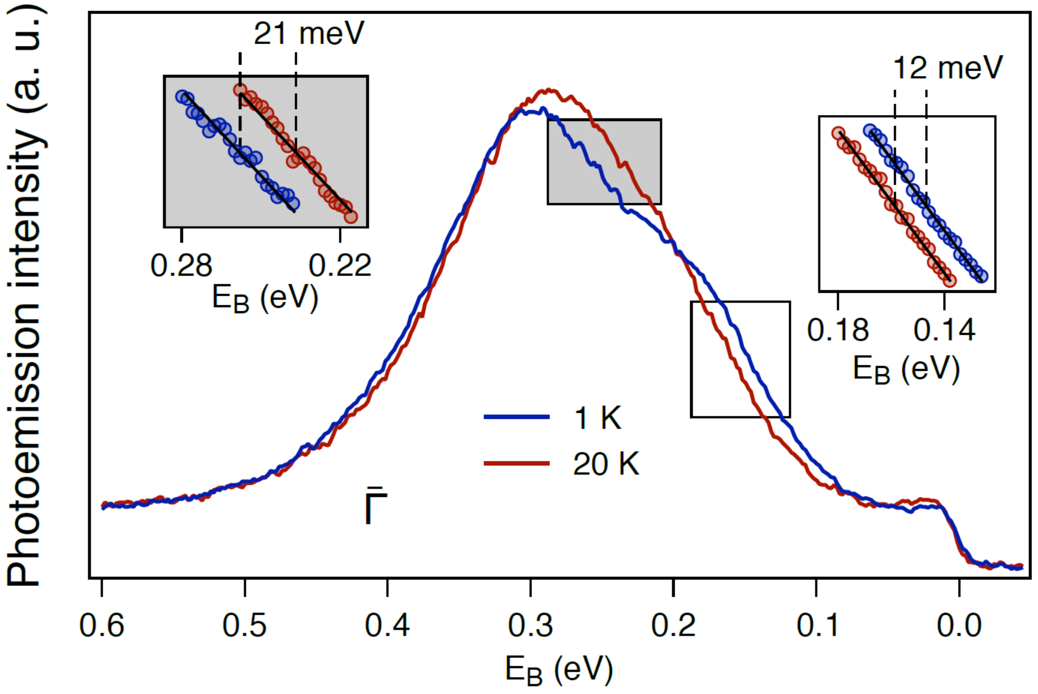
J. Sanchez-Barriga et al,. Nature Comm. 7:10559 (2015).

Electronic structure

ARPES BESSYII, HZB Berlin, Bi_2Te_3 6% Mn doped samples







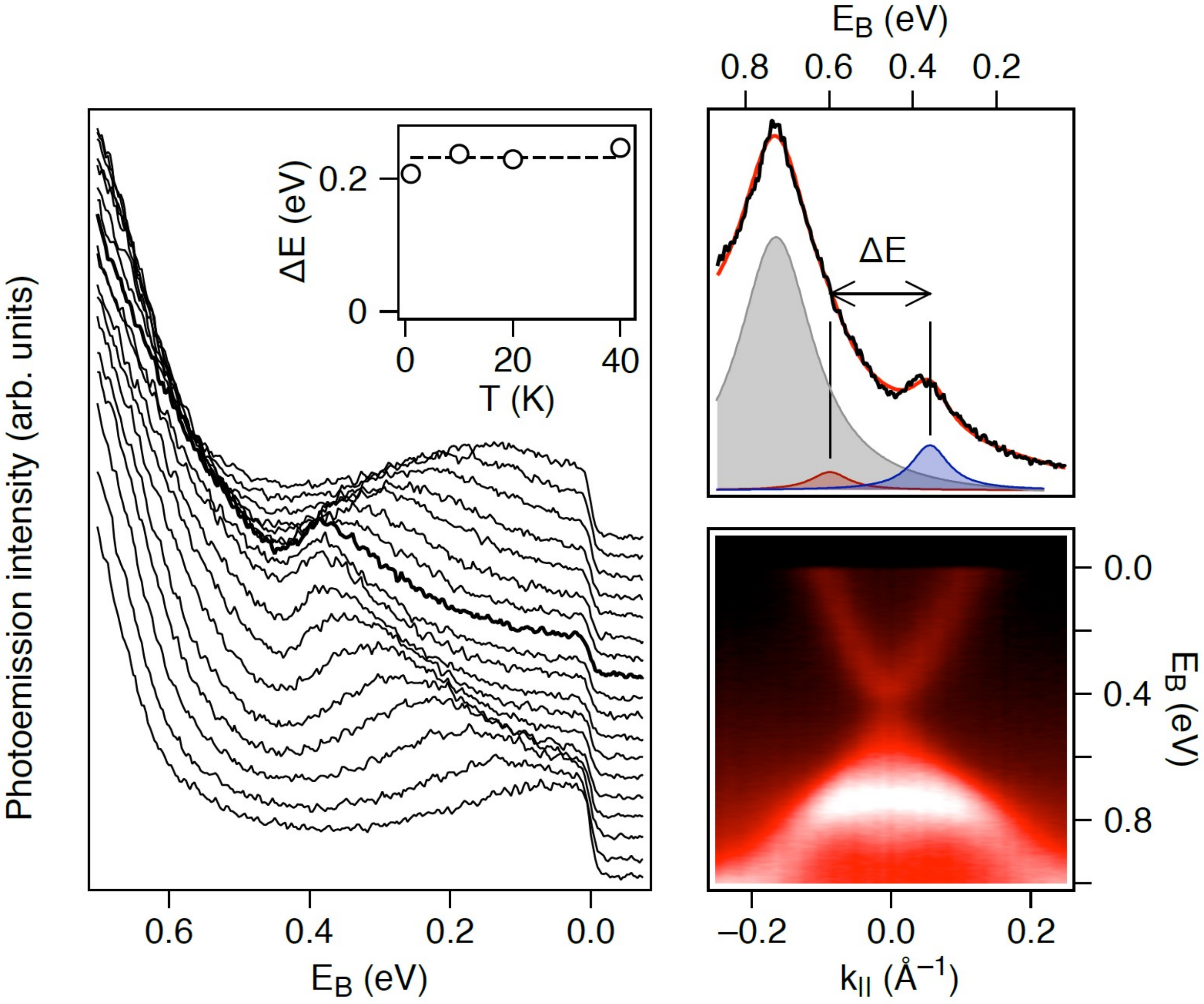
Magnetic gap 90 meV

DFT theoretical prediction
≈16 meV for 10% Mn
Henk et al., Phys. Rev. Lett **109**, 076801 (2011).

≈40-80 meV for heterostructure
Otrokov et al., 2D mater. **4**, 025082 (2017).

Electronic structure

6% Mn doped Bi_2Se_3 at 1K



Temperature
independent
nonmagnetic
gap 200 meV

Conclusion

- Mn doped topological insulators form natural heterostructure of alternating QL and SL segments
- Mn atoms are mostly positioned in the central position of septuple layer
- Ferromagnetic ordering has been observed with Curie temperature in range of 6K to 15K for Mn concentration above 3%
- Easy magnetization axis is:
  - Out-of-plane for bismuth telluride
  - In-plane for bismuth selenide
- Bismuth telluride shows large magnetic band gap of (90±10) meV opened bellow Curie temperature
- Bismuth selenide does show temperature independent band gap of ≈200 meV

Topologické izolátory dopované Mn

Závěr:

určili jsme strukturu vrstev, uspořádání Mn

Feromagnetické pod cca 15K

Směr snadné magnetizace kolmo k povrchu (telurid), v rovině (selenid)

Pozorován gap v pásové struktuře indukovaný feromagnetickým přechodem