Structural and electronic properties of Mn doped topological insulators Bi_2Te_3 and Bi_2Se_3

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Outline

- Motivation
- Mn doped topological insulators thin films
  - sample preparation
  - structure: XRD, XAFS, HRTEM
  - magnetic properties
  - elektronic structure: ARPES
- Conclusion

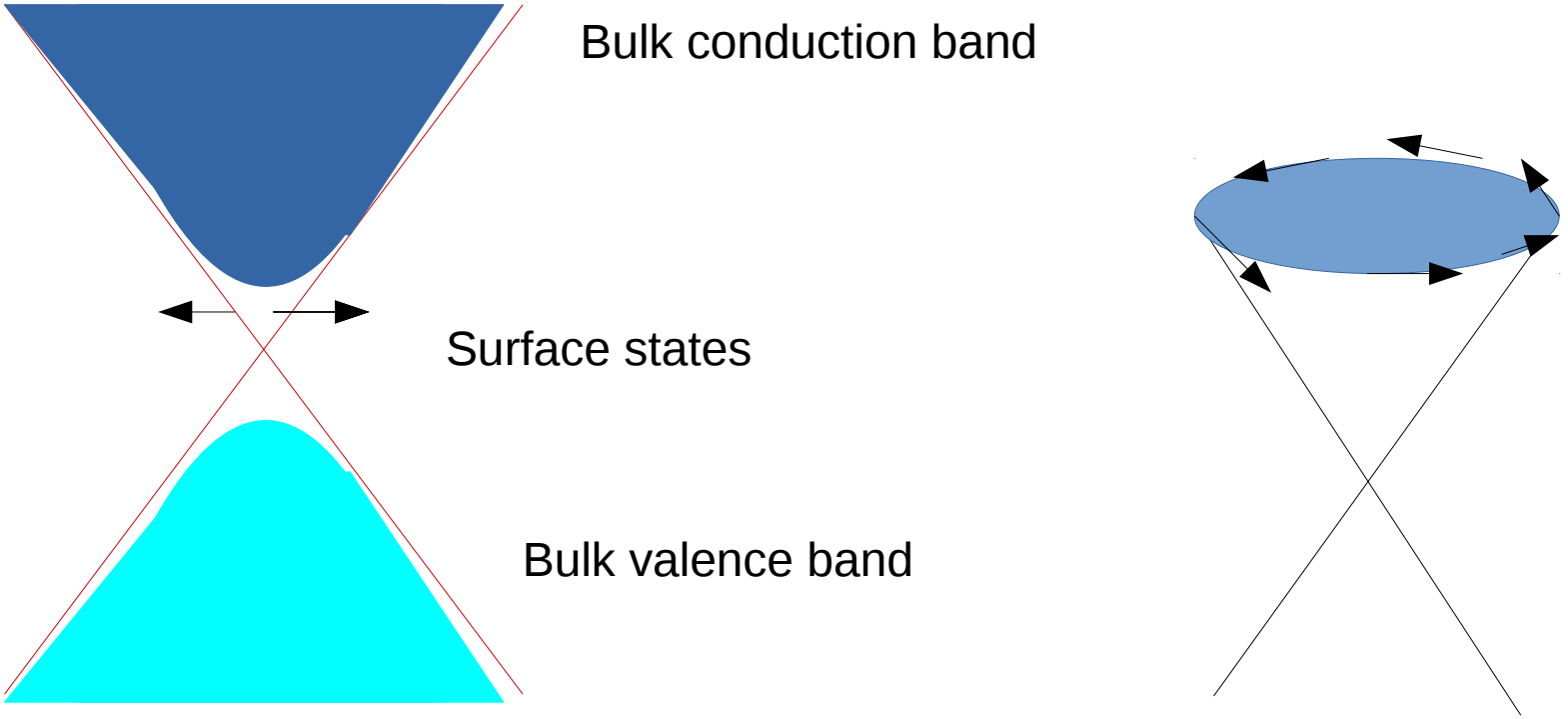
Topological insulators

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

Sample preparation

G. Springholz group, JKU Linz

Mn doped Bi_2X_3
thickness 300 to 500nm

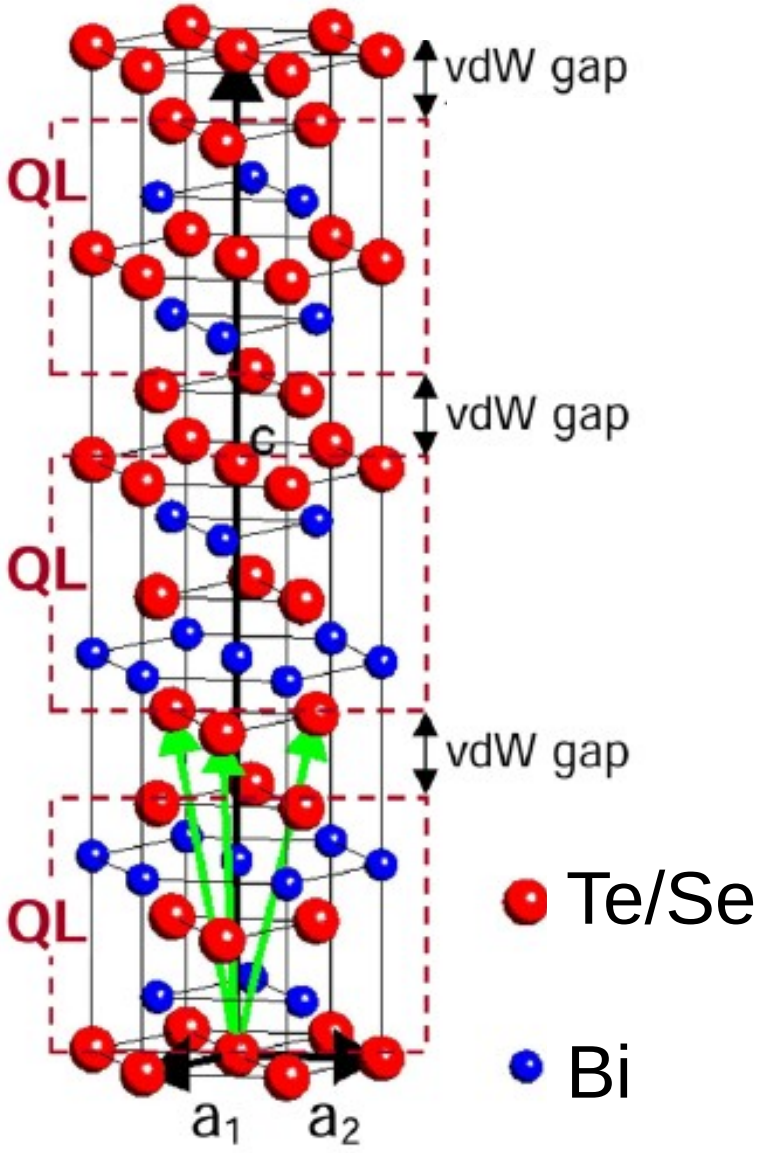
Substrate BaF_2 (111)

Deposition technique:
Molecular beam epitaxy

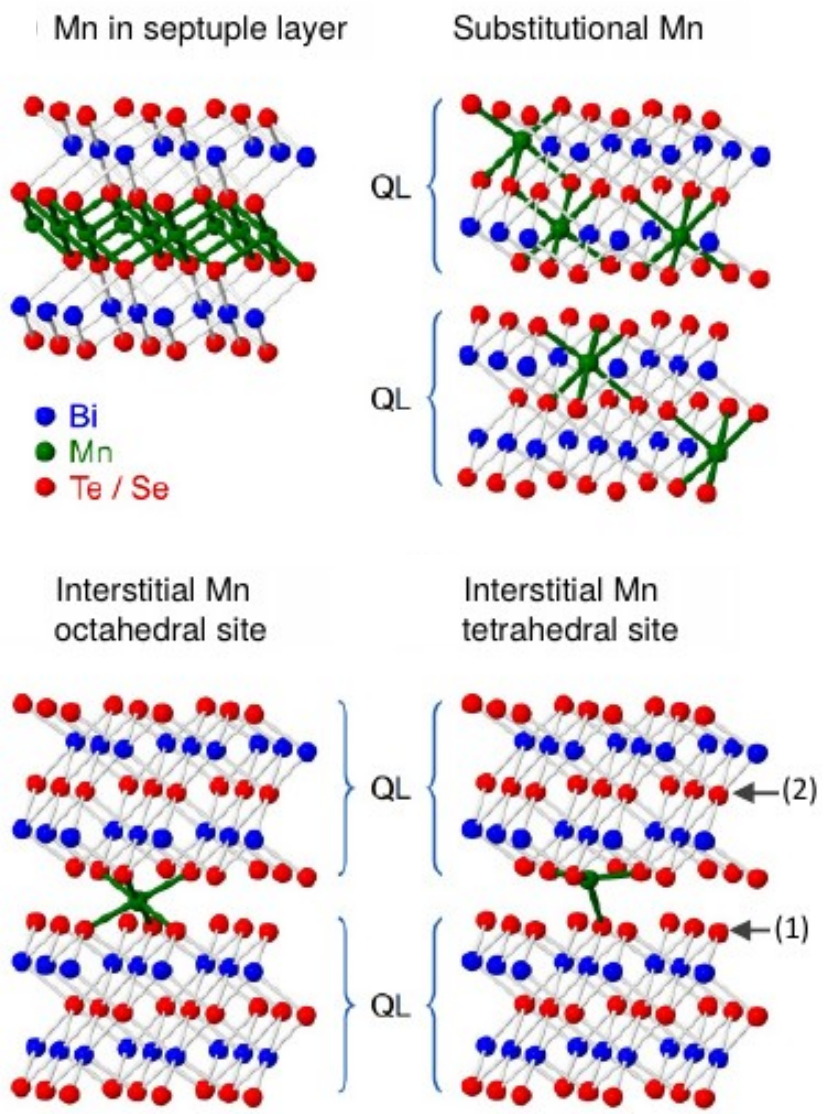
Compound sources:
Bi_2Te_3/ Bi_2Se_3, additional Te/Se cell to achieve correct stoichiometry

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

Crystal structure of Bi_2X_3 (X=Se,Te)



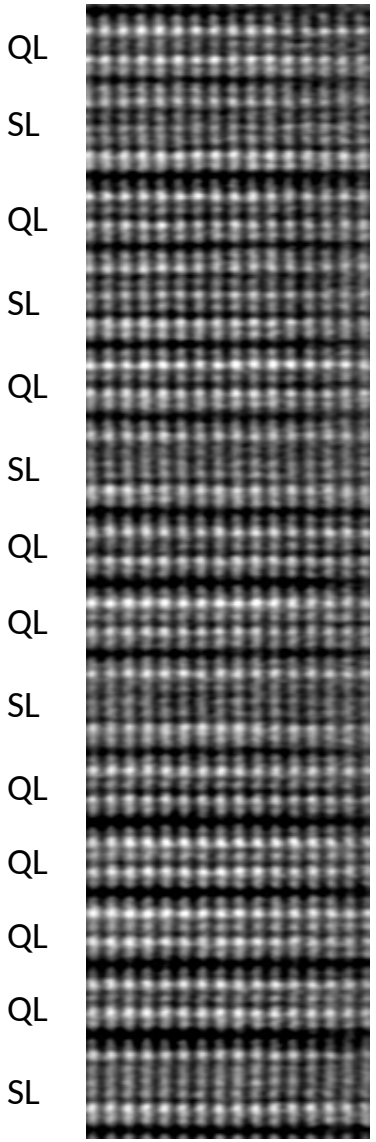
Possible incorporation position of Mn atoms



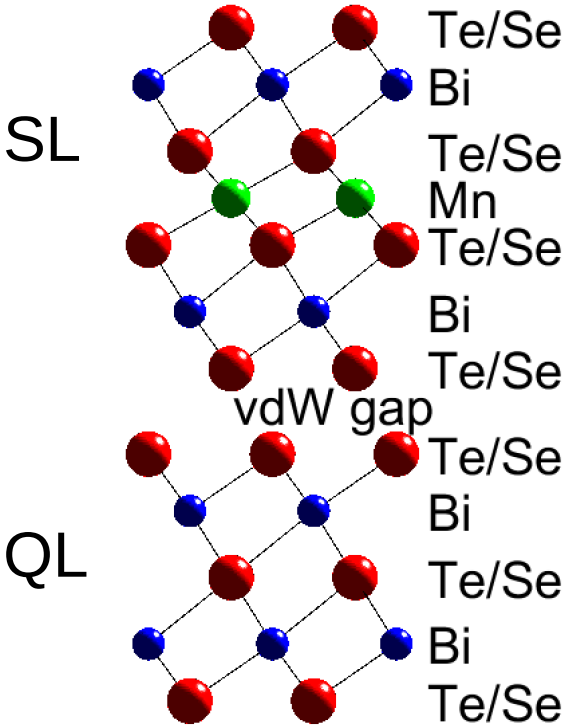
Electron microscopy

JKU Linz, Graz

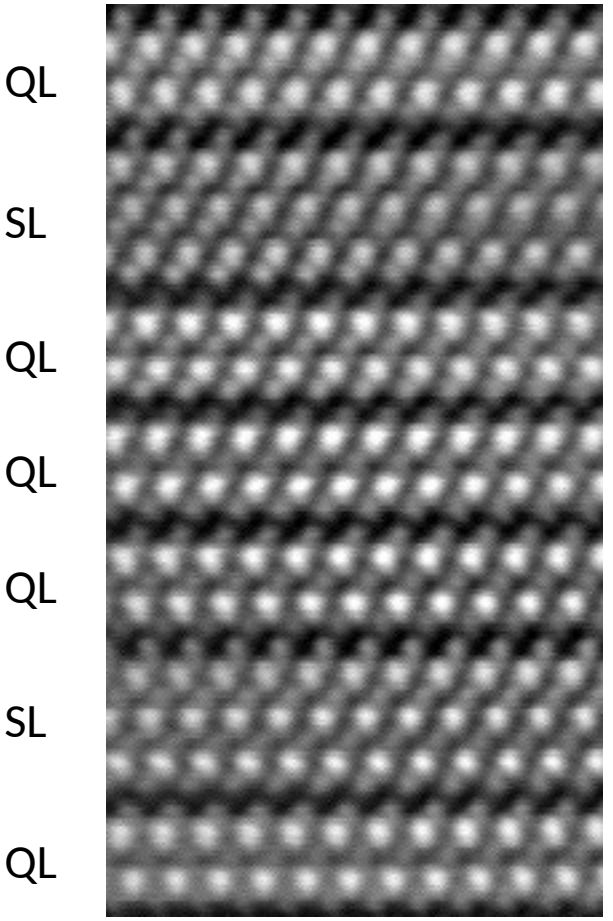
10% Mn Bi_2Te_3



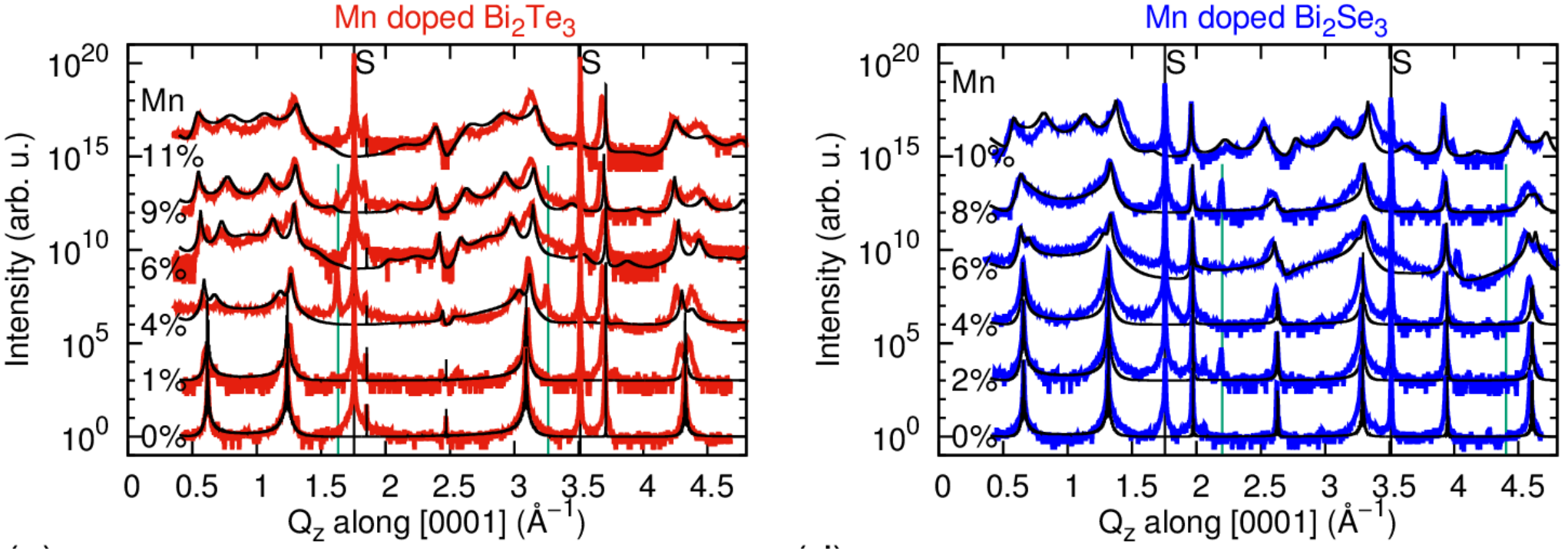
HAADF STEM



6% $MnBi_2Se_3$



XRD structure analysis



Symmetric scan with scattering vector perpendicular to the surface

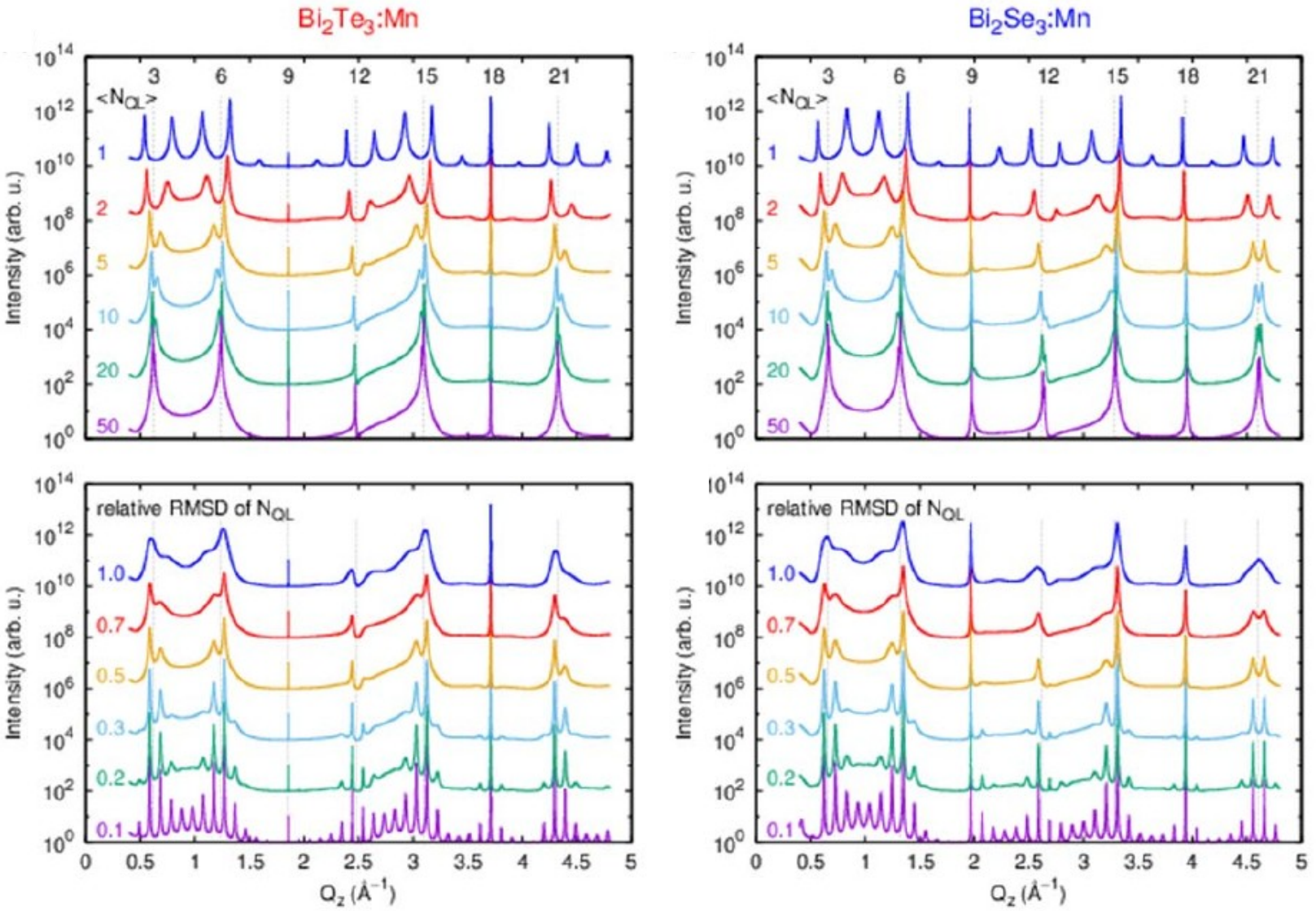
Higher Mn content leads to disturbed structure

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

XRD structure analysis

Paracrystal model parameters:

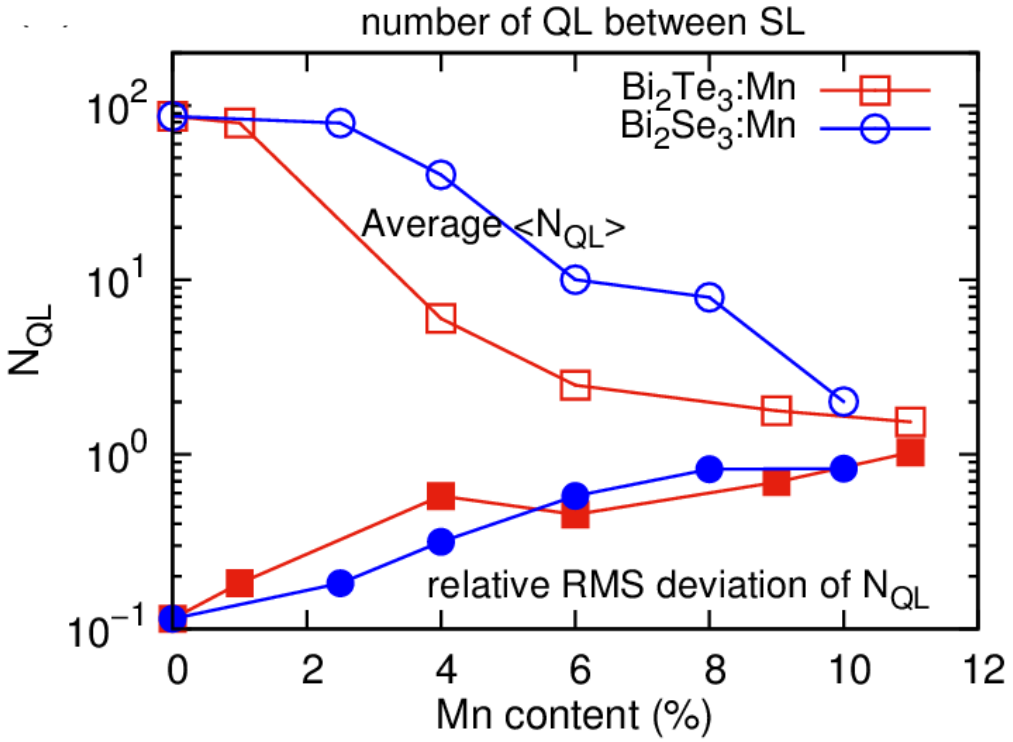
average length and RMSD of QL and SL segments

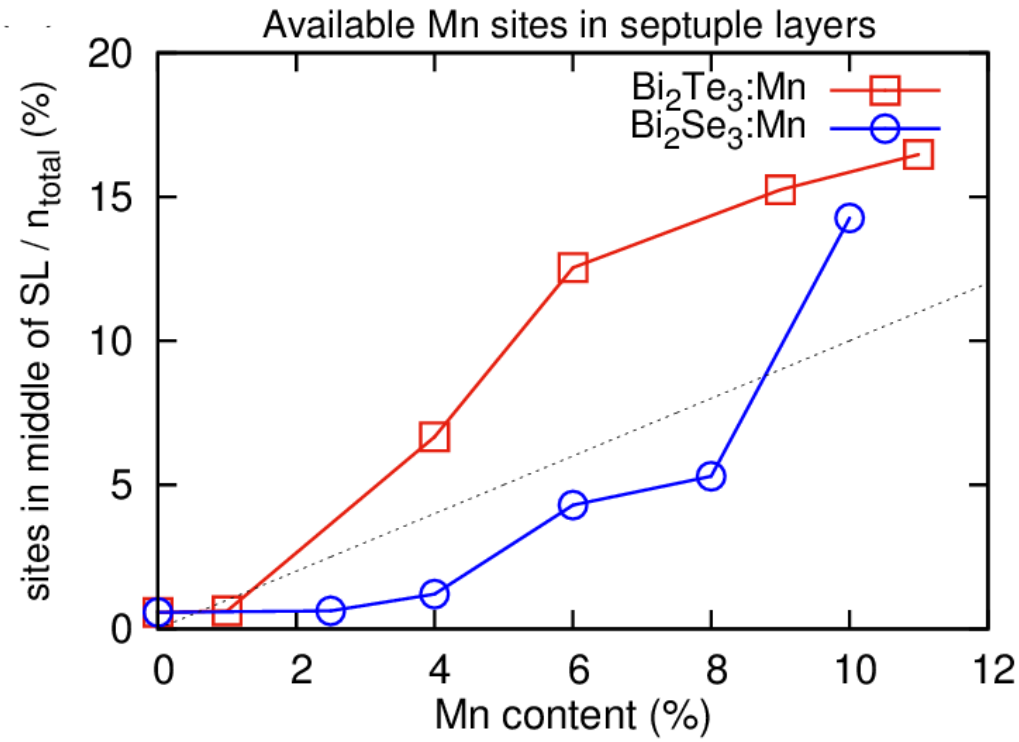


relative RMSD =0.5

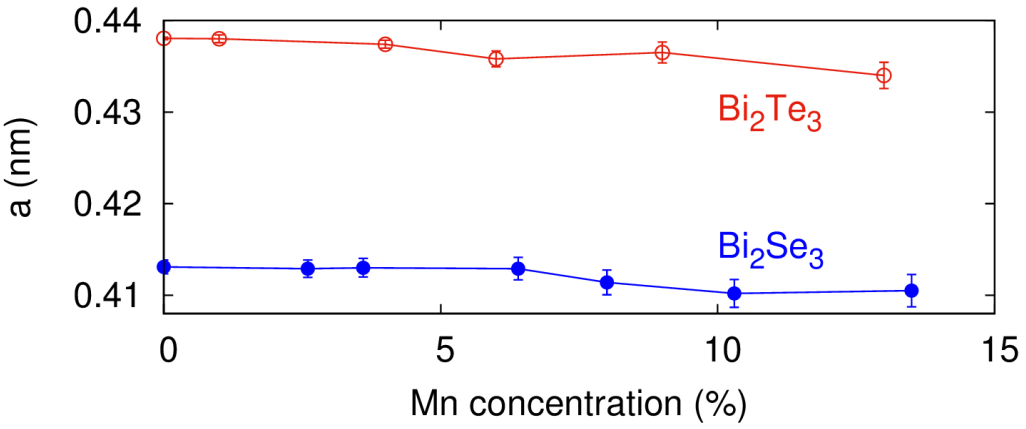
$\langle N_{QL} \rangle$=5

XRD structure analysis



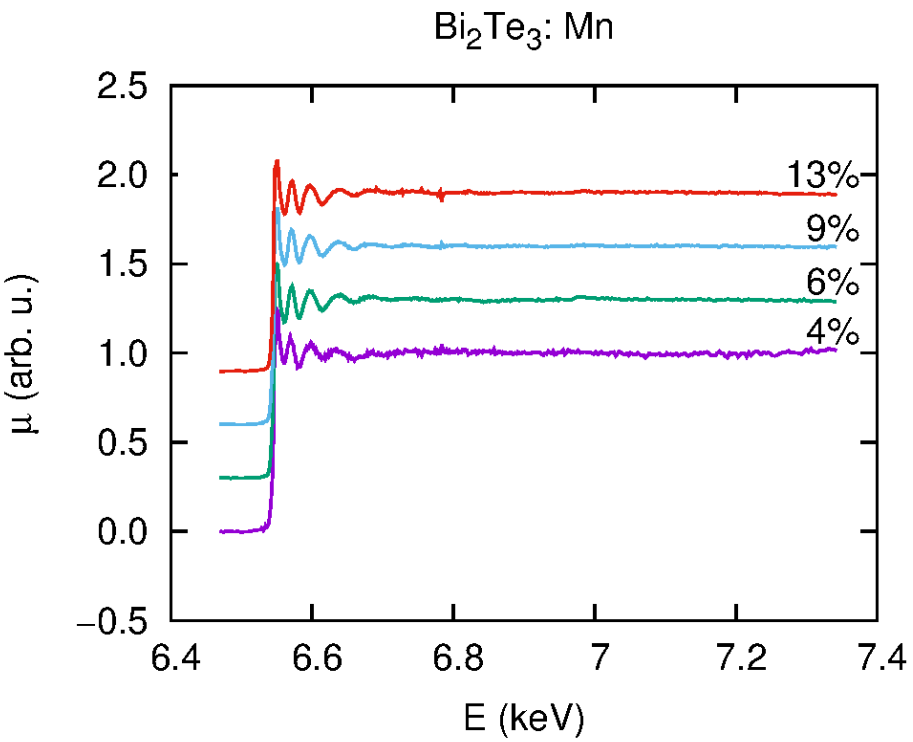


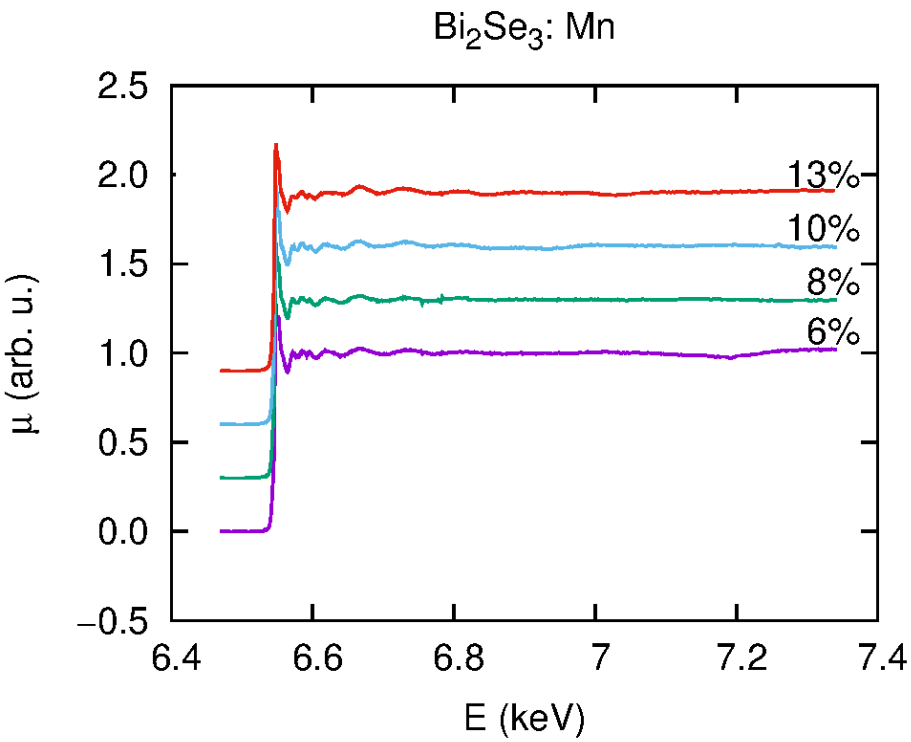
In-plane lattice parameter dependence



X-ray absorption spectroscopy

Experiment at BM23, ESRF Grenoble

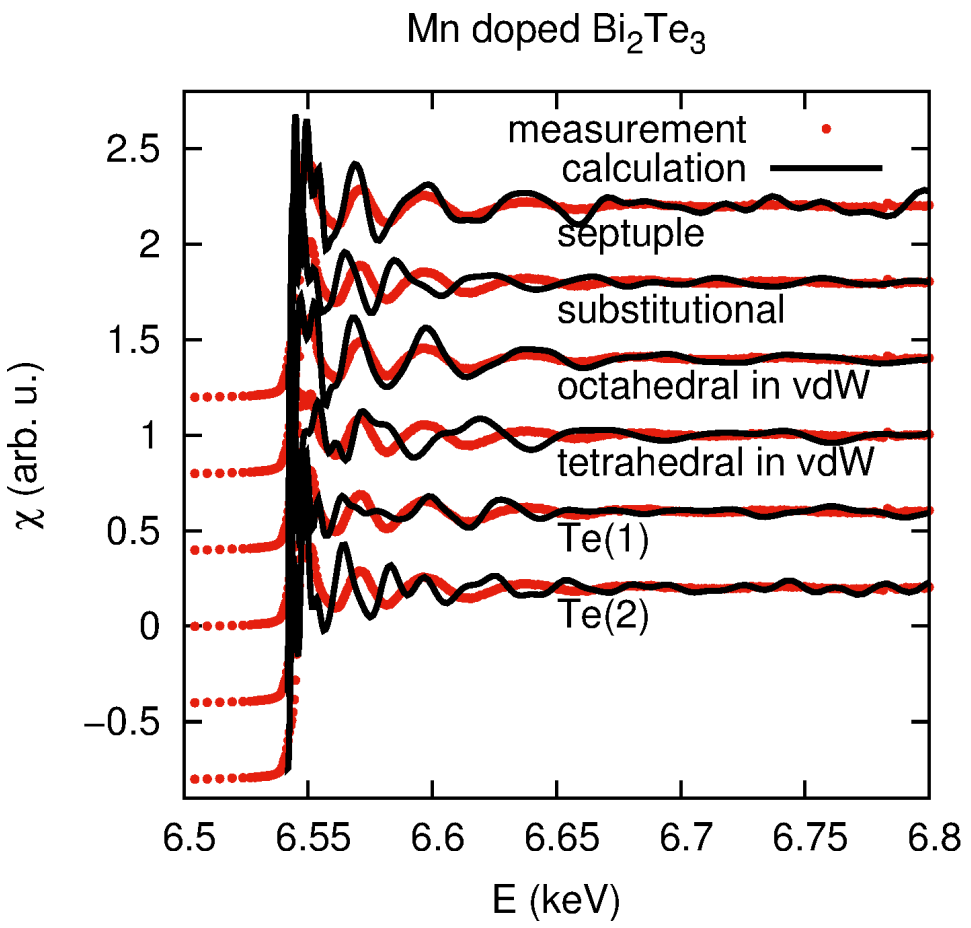


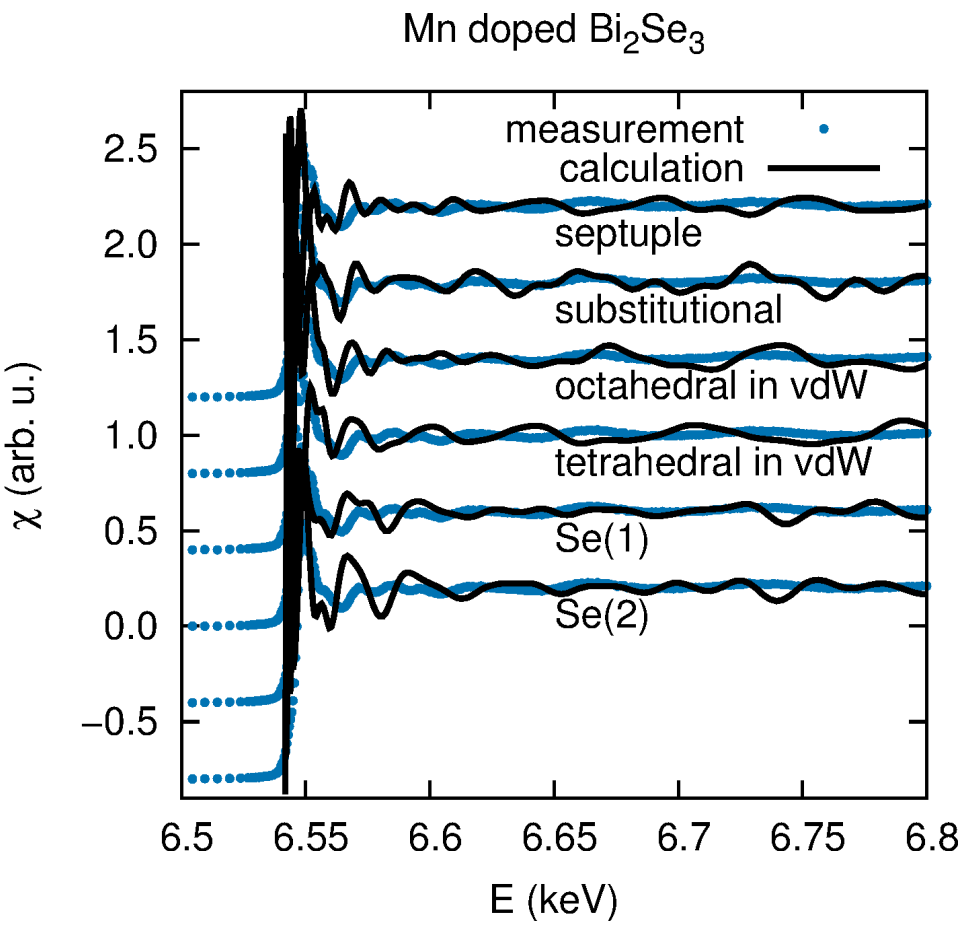


Very weak Mn concentration dependence

X-ray absorption spectroscopy

Simulations of various Mn positions

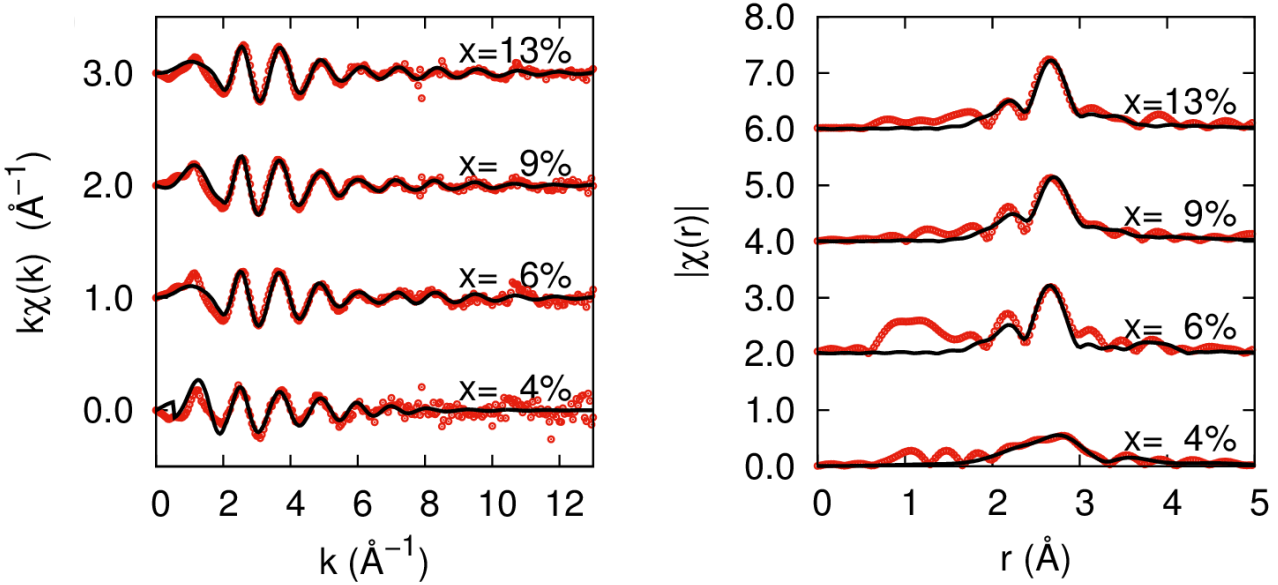




X-ray absorption spectroscopy

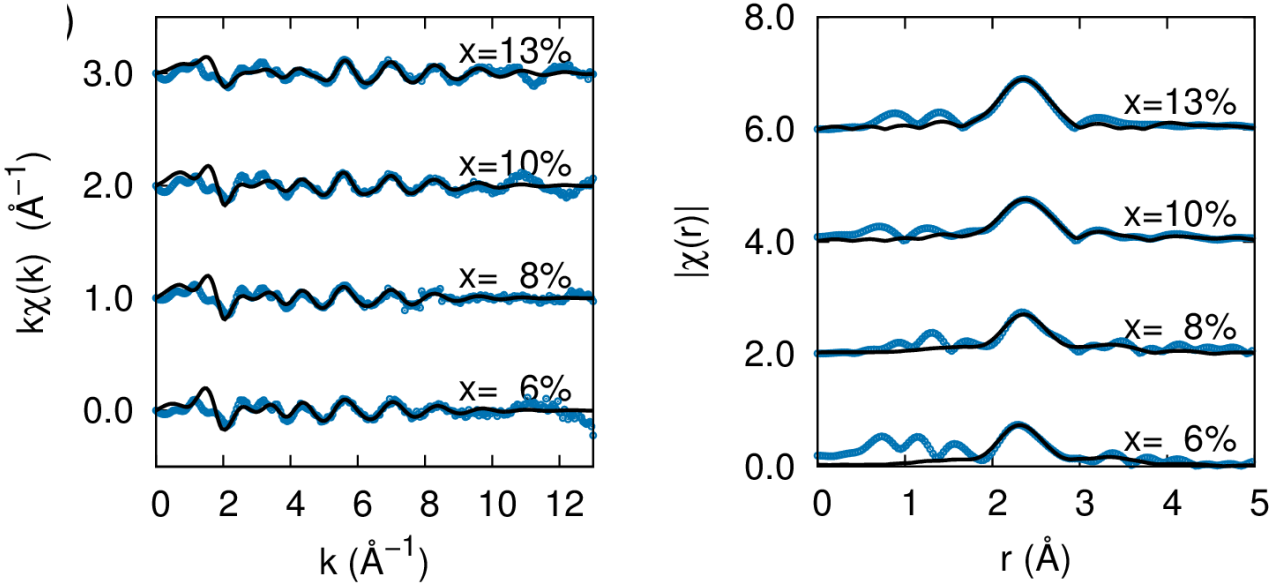
Fitted distances of Mn nearest neighbors

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

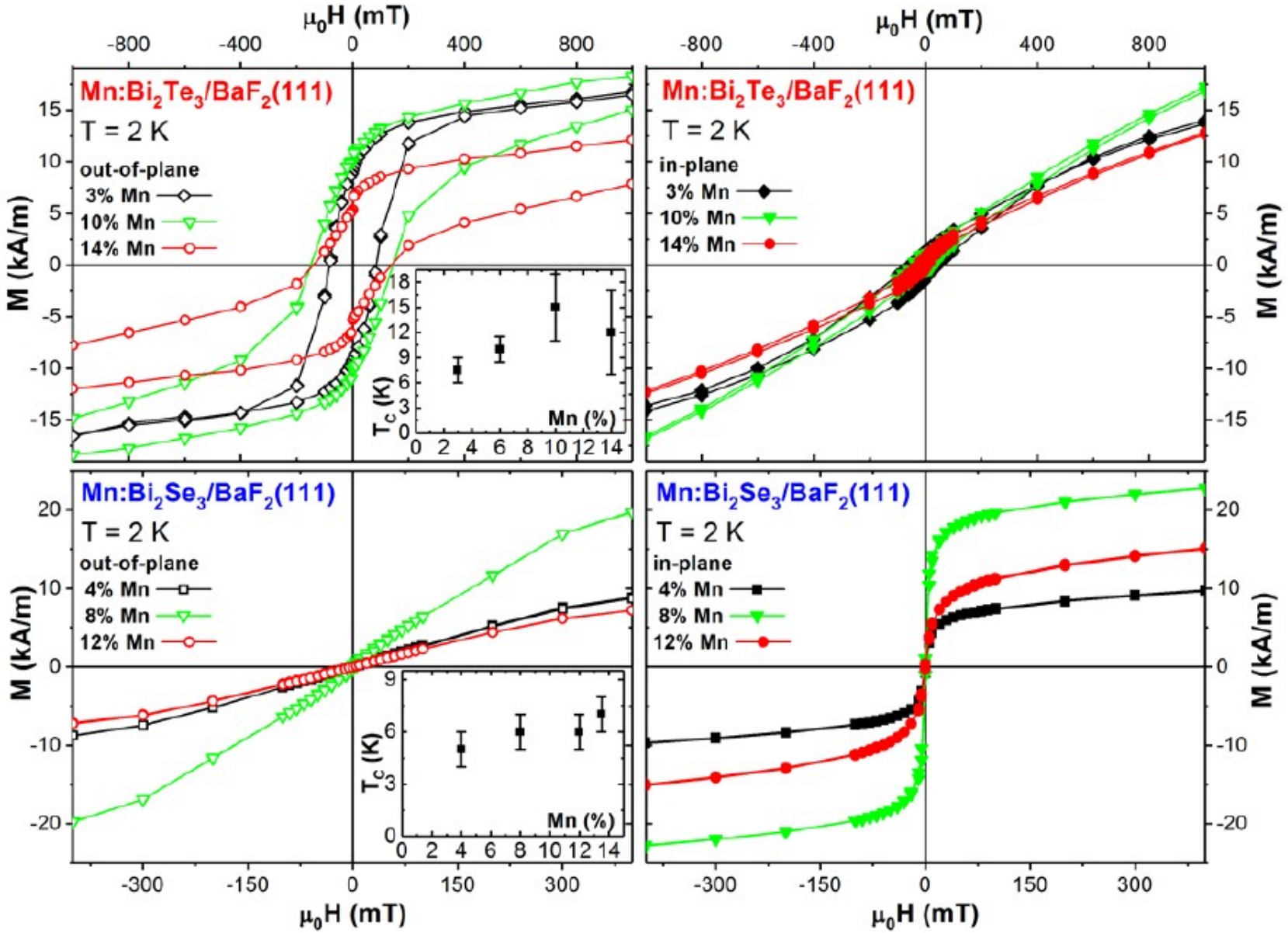
Mn doped Bi_2Se_3



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

Magnetic properties

SQUID (JKU Linz)

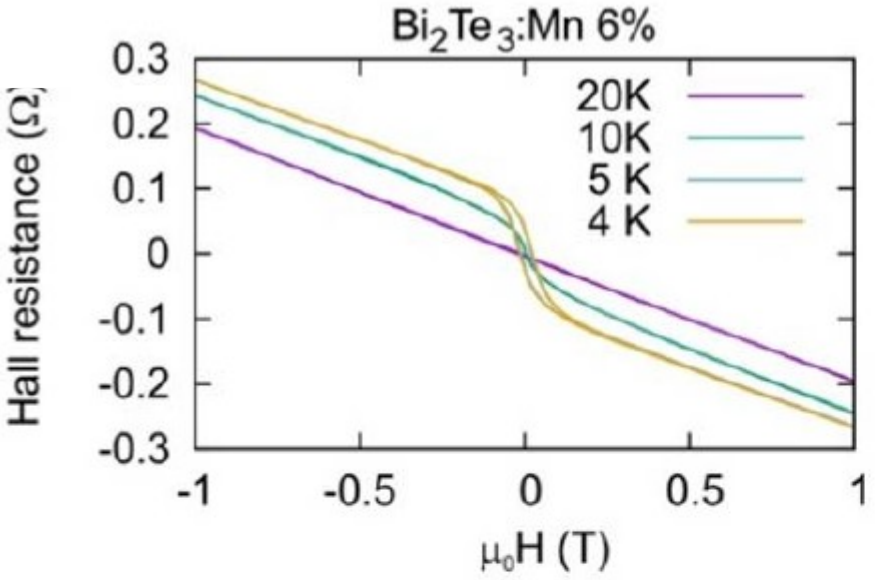


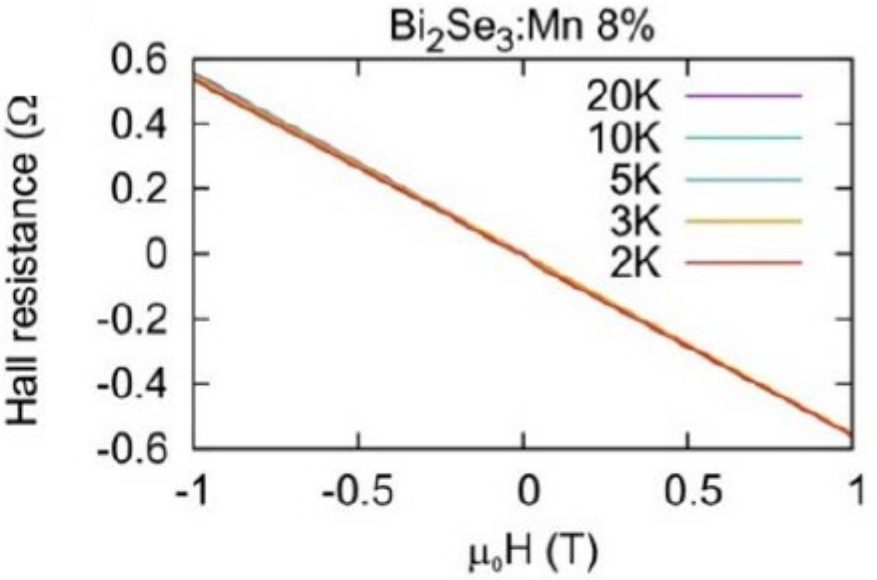
Telluride
easy axis
out-of-plane
$T_C \approx 10$ K

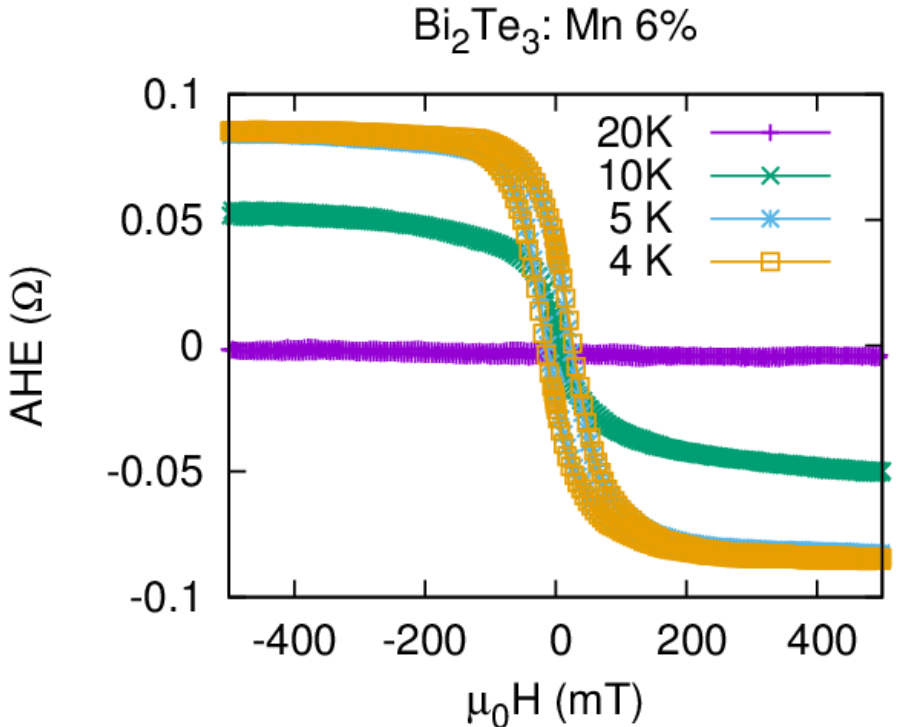
Selenide
easy axis
In-plane
$T_C \approx 6$ K

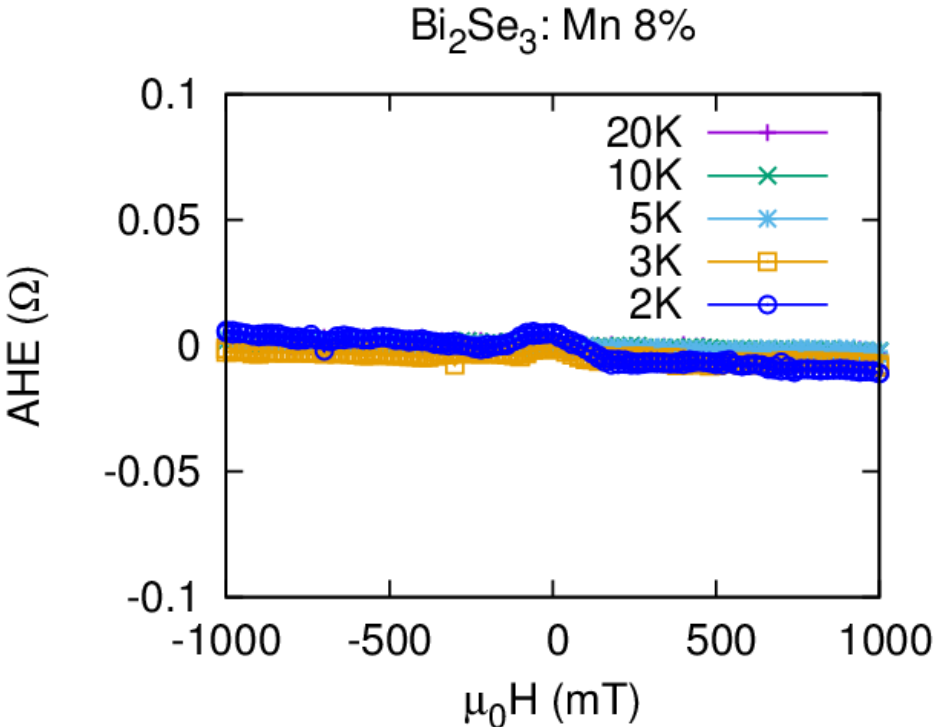
Transport measurements

Hall effect in van der Pauw geometry





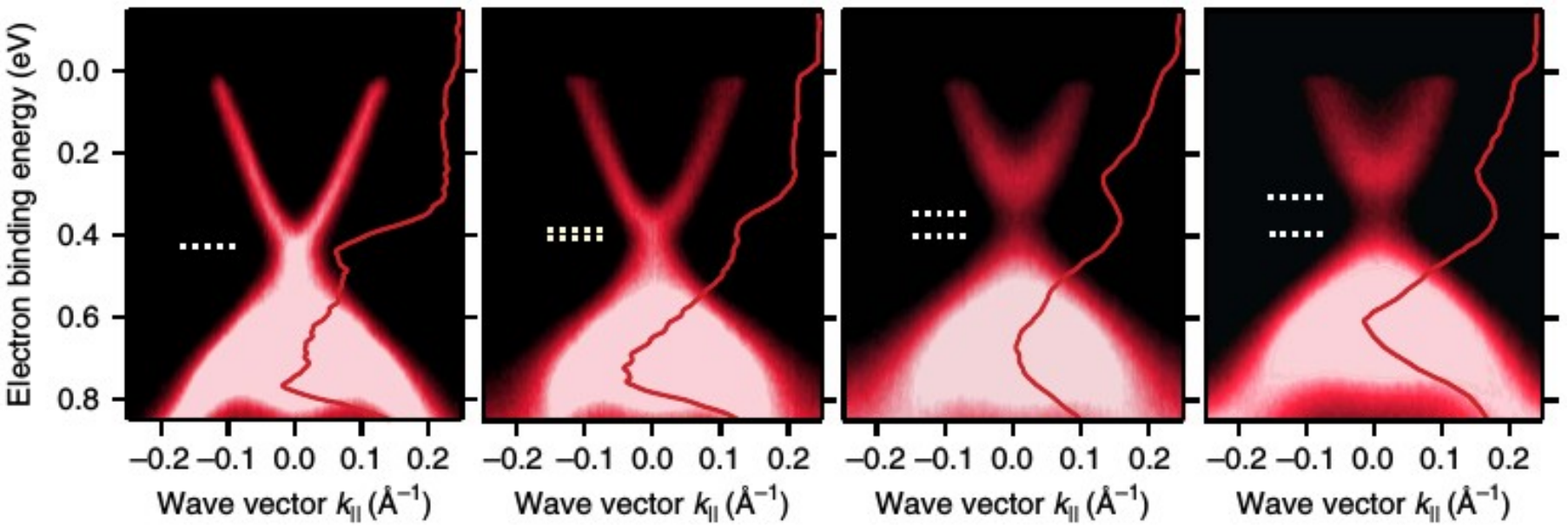




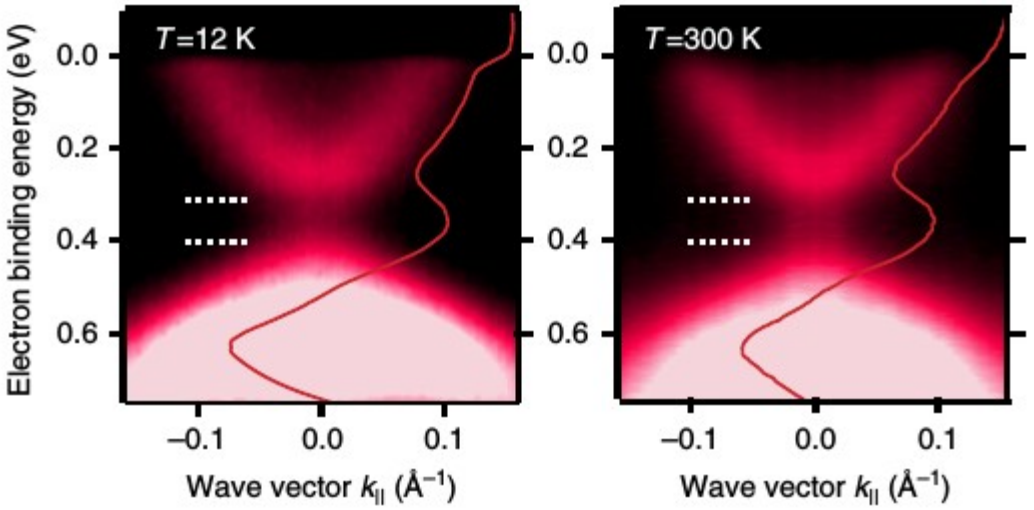
Electronic structure

ARPES BESSYII, HZB Berlin Bi_2Se_3, 12K

Mn 0% 2% 4% 8%



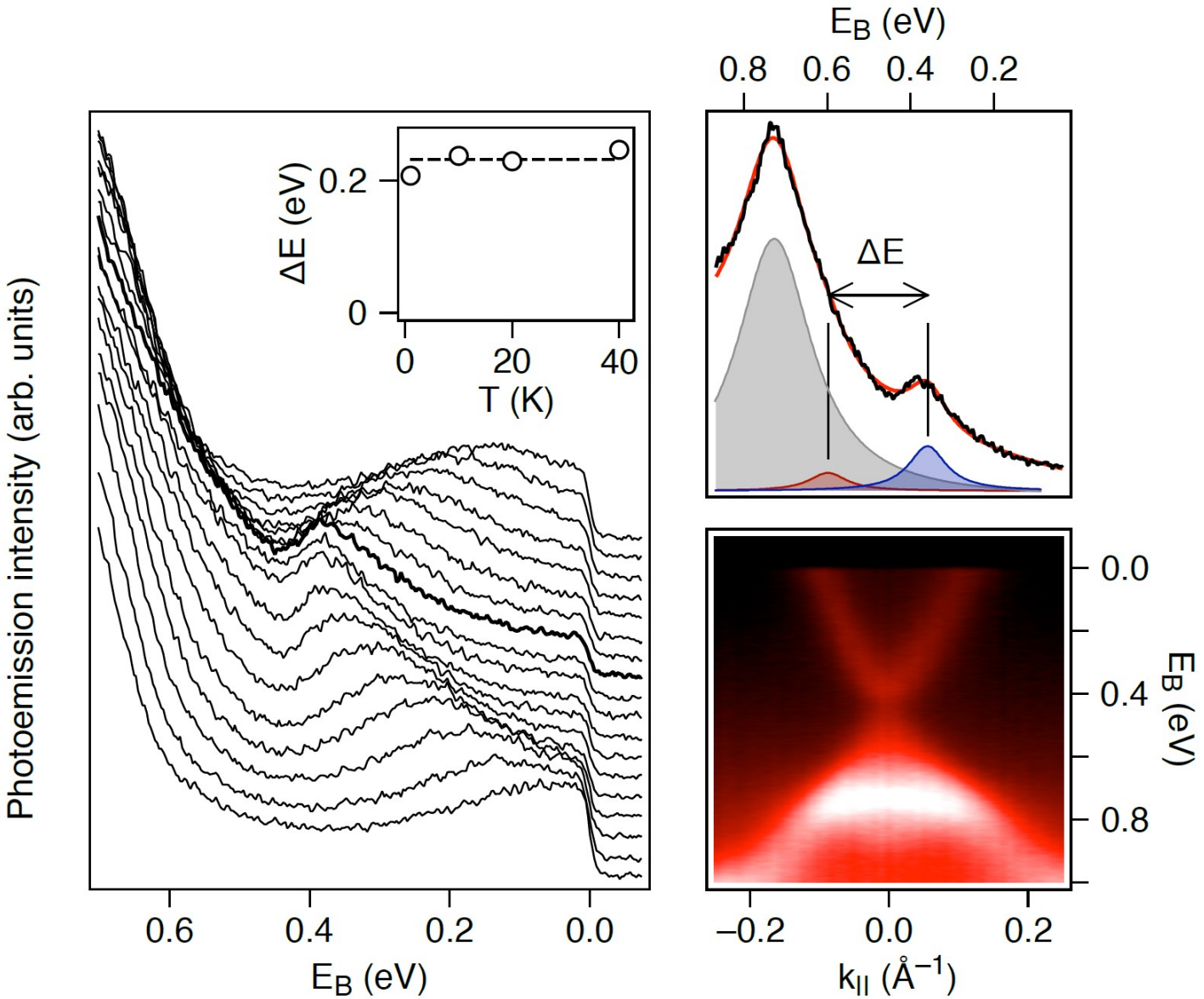
Mn 8%



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

Electronic structure

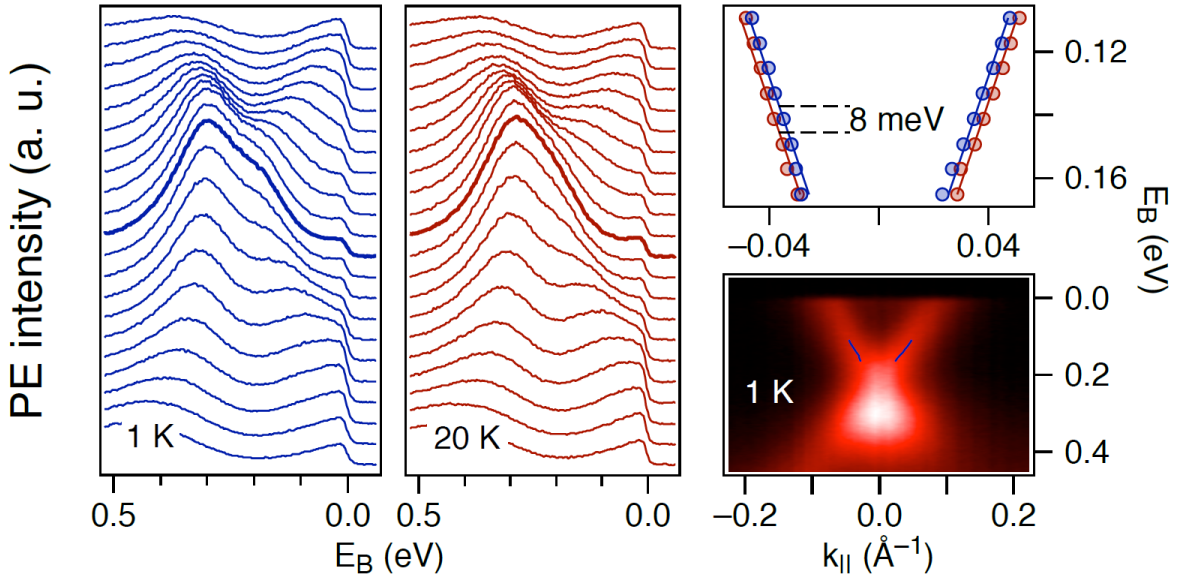
6% Mn doped Bi_2Se_3 at 1K

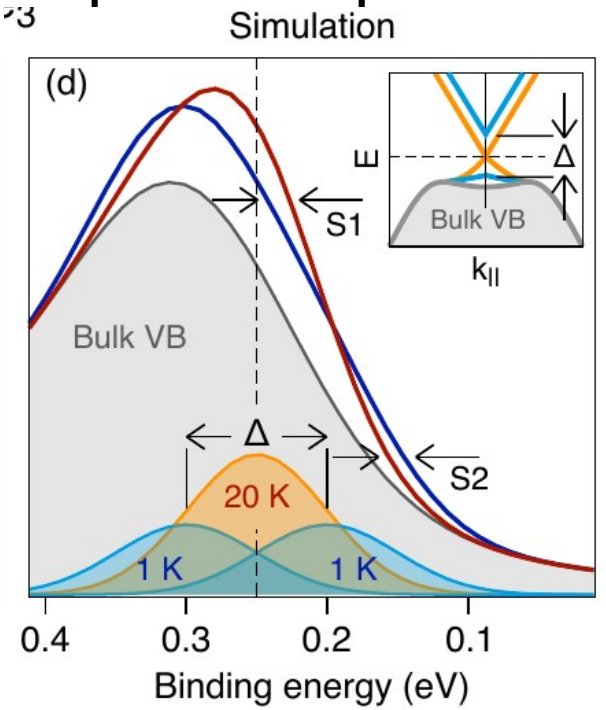


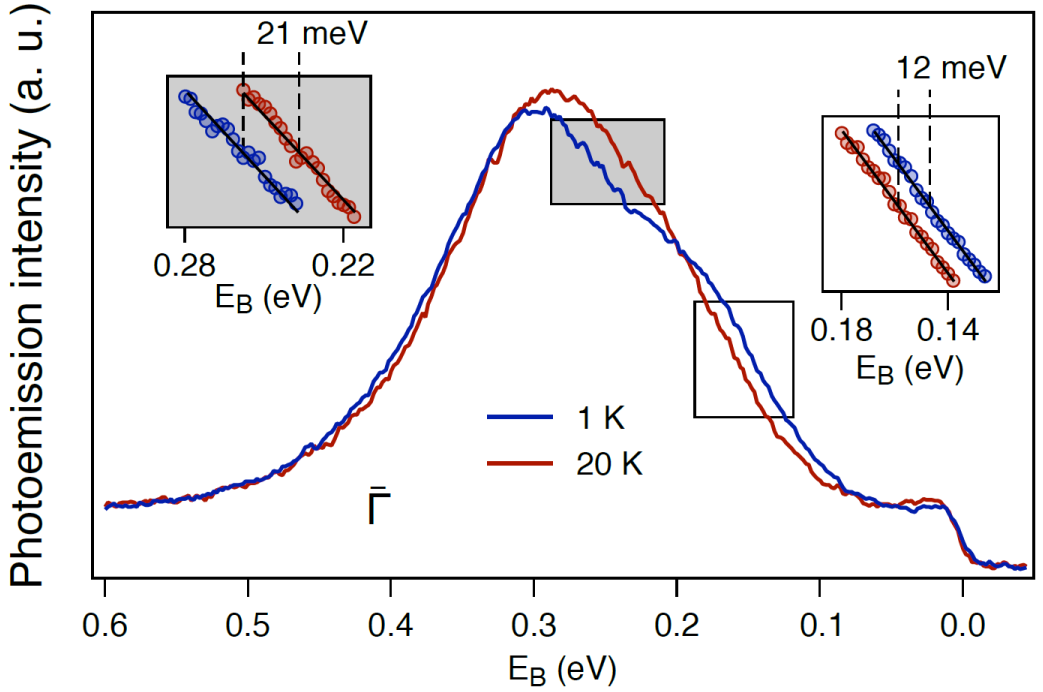
Temperature independent nonmagnetic gap 200 meV

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).

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

Transport measurements

Hall effect in van der Pauw geometry