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Local structure of transition metal dopants into 3D topological insulators probed with angular dependent XAFS

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A new state of quantum matter which has a topologically nontrivial electronic structure characterized by a bulk energy gap but gapless chiral edge states, leading to the quantized Hall effect without an external magnetic field is among most intriguing physical phenomena discovered in the last decade. Quantum anomalous Hall effect has been observed in thin films of V and Cr doped topological insulators (TIs), i.e. magnetic topological insulators, where robust bulk ferromagnetic (FM) ordering is spontaneously developed. The ability to externally control the magnetic properties of TIs could be important both for fundamental and technological interest, particularly in view of recent developments in magnetoelectrics and spintronics [1].

Among crystalline TI the long range magnetic order is established only in the Mn-doped Bi₂Te₃ in the temperature range below T_C = 12 K. On the other hand, in iron and cobalt doped bismuth chalcogenides, long range magnetic order has not been observed, while magnetic susceptibility reveal intriguing anisotropy, that is tentatively ascribed to non-uniform distribution of transition metal dopants between cation sites of Bi and interstitial position within Van der Walls gap.

In this contribution we present results of systematic investigations of local structure around transition metal dopants into single crystals of bismuth chalcogenides by means of K-edge EXAFS and angular dependent XANES spectra. The measurements performed at room temperature at SuperXAS beamline show e.g. a systematic angular dependence in Mn doped Bi₂Te₃, while the evolution of respective spectra in Mn doped Bi₂Se₃ is negligible. A significant difference between these systems is also visible in EXAFS spectra that reveal considerable evolution in local crystal structure around Mn dopants in both systems. Supported by theoretical modeling of angular dependent XANES by means of FDMNESS code and double shell analysis of EXAFS spectra, we will assess the preferential sites for transition metal doping of TI crystals and discuss its influence on magnetic properties of magnetic crystalline TIs.

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