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ATOMIC STRUCTURE AND PROPERTIES OF MAGNETIC ADSORBATES ON THE TOPOLOGICAL INSULATOR Bi_2Se_3

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Topological insulators (TI) represent an unusual state of matter. While they are insulators in the bulk they are metals at the surface. Tremendous interest has arisen in the recent past primarily focused on the study of the electronic and transport properties of uncovered and adsorbate covered TI's. The latter is motivated by the question whether the topological state is robust against adsorption of magnetic and non-magnetic adsorbates [1,2]. By contrast, atomically resolved structure studies relating electronic properties to the geometric structure are hardly available.

We have carried out combined experimental and theortical studies on uncovered and adsorbate covered Bi_2Se_3(0001) after *in-situ* deposition of ultra-thin films of Fe and Cr. We have analyzed the atomic structure by surface-x-ray diffraction, in combination with scanning tunneling microscopy/spectroscopy (STM/STS), and angular resolved photoemission (ARUPS). Experiments were complemented by *ab-inito* calculations. Our investigations have revealed many unexpected results. This presentation gives an overview over some of them. For instance:

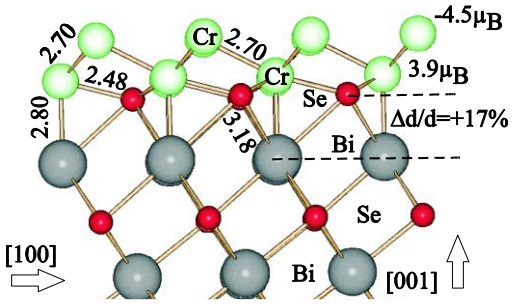

Fig. 1. Model of the structure of Cr on Bi_2Se_3(0001). Distances in Å, magnetic moments in μ_B.

(i): The top layer spacing (Se/Bi) of bare bulk Bi_2Se_3(0001) shows an expansion in the 2-10 percent range relative to the bulk. This depends on the (very small) amount of carbon contamination always present in bulk samples. ARUPS and theory confirm the concomitant shift of the bulk states relative to the (intact) Dirac cone. **(ii)**: Adsorbed Cr-atoms reside in threefold hollow sites next to surface Se atoms (Fig.1) and form a distorted hexagonal overlayer which is ferrimagnetic ($T_C \approx 50$ K) with an in-plane easy axis magnetization as confirmed by Magnetooptic Kerr effect (MOKE) experiments and theory. **(iii)**: Fe adsorption at room temperature in the monolayer range induces an approx 20-30% Fe/Bi substitution within the first quintuple layer. At elevated temperatures (T>140°C) the formation of a ≈15 Å thick orthorhombically distorted FeSe film sets in. Its lattice parameter is compressed by 5% relative to the tetragonal bulk structure (3.56 Å vs. 3.77 Å) along one in-plane axis. STS shows signatures linked to superconductivity up to T=30 K at least. In all studies no substantial fraction of intercalated atoms within the first van-der-Waals gap is found.

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[1] L. A. Wray, S.Y. Xu, Y. Xia, et al. *Nature Phys.*, **7** (2010) 32.

[2] T. Valla, Z.-H. Pan, D. Gardener, Y.S. Lee, and S. Chu, *Phys. Rev. Lett.* **108** (2012) 117601.