MS13-1-11 Symmetry, Structural and Electronic Correlations in a Family of Bismuth-based Layered Materials #MS13-1-11

E. Carrillo-Aravena [1], A. Consiglio [2], J. Heßdörfer [3], R. Friedrich [3], D. Di Sante [4], M. Ruck [5]
[1]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat - Dresden (Germany), [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat - Würzburg (Germany), [3]Experimentelle Physik VII, Universität Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat - Würzburg (Germany), [4]Center for Computational Quantum Physics, Flatiron Institute - New York (USA), Institut für Theoretische Physik und Astrophysik, Universität Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat - Würzburg (Germany), [5]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Max Planck Institute for Chemical Physics of Solids and Würzburg-Dresden Cluster of Excellence ct.qmat - Dresden (Germany)

Abstract
Topological insulators (TIs) are semiconductors with protected electronic surface states that allow dissipation-free transport. They are proposed as ideal materials for spintronics and quantum computing.
The first verified 3D weak TI, $Bi_{12}Rh_3I_9$[1-5], consists of two types of alternating charged layers. The anionic layer of edge-sharing $[Bi_2I_8]^{2-}$ octahedra and the topological non-trivial layer $[Bi_{12}Rh_3I]^{2+}$ (**Figure 1**). The latter determines the electronic states with inverted parity around the Fermi level and consists of a net of edge-sharing Rh-centred Bi cubes forming a prismatic rhombitrihexagonal honeycomb lattice, with an iodide ion at the centre of each hexagonal prism.
The TI layer has been observed in the structurally similar, but topologically trivial compounds $Bi_{13}Pt_3I_7$[6,7] and $Bi_{12}Pt_3I_5$[7] that contain a different spacer, stacking sequence and electron count. Therefore, it was found that the anionic spacer played a decisive role in defining whether the topological properties of the material would be trivial or not.
Herewith, we present the structure and properties in a series of layered materials derived from those mentioned above: $Bi_{12}Rh_3Cu_2I_5$(**1**)[8] (**Figure 2**), $Bi_{12}Rh_3Ag_2I_5$(**2**), $Bi_{12}Pt_3CuI_5$(**3**), $Bi_{12}Pt_3AgI$(**4**) and $Bi_{12}Rh_3Ag_6I_9$(**5**). For those compounds, the TI layer is left unchanged, while the spacer layer is substituted for studying its impact on the topological properties. Full-relativistic DFT studies in conjunction with ARPES have shown a relationship between the size of the bulk bandgap and the thickness and chemical nature of the spacer layers. Structural characterization of these materials is challenging not only because of stacking faults — intrinsic to their layered structure — but also atomic disorder within the spacer layers. Furthermore, twinning by pseudo-merohedry is common for **1**, **2**, **3** and **4**, all of which share highly specialized metrics close to a hexagonal cell, but orthorhombic or monoclinic space groups.

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Figure 1: TI layer $[Bi_{12}M_3I]^{x+}$ (M = Rh, Pt), overlaid with its layer group symmetry *p*6/*mmm*.

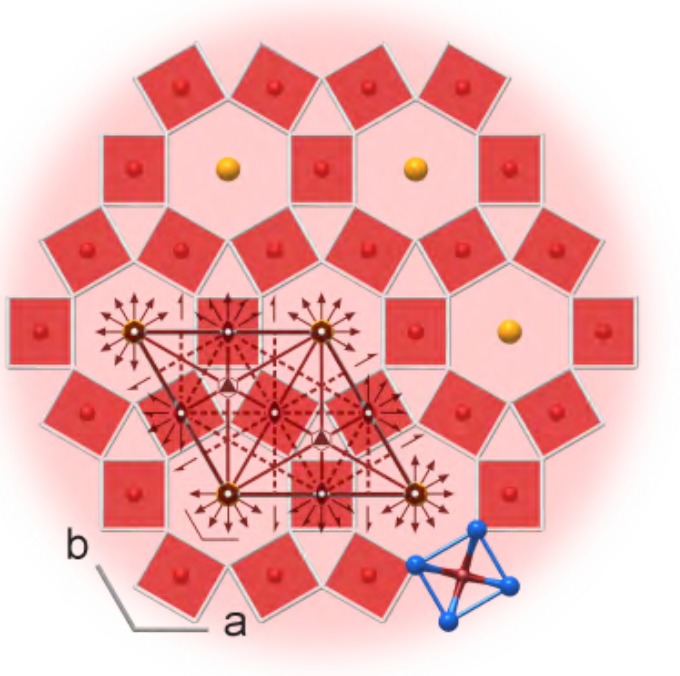

Figure 2: Crystal structure of the 3D weak TI $Bi_{12}Rh_3Cu_2I_5$. It consists of TI layers $[Bi_{12}Rh_3I]^{2+}$ separated by topologically trivial iodidocuprate(I) groups.