H2020 FET-Open Research and Innovation Actions Project Number 766566
Antiferromagnetic spintronics (ASPIN)

Work package 1, Deliverable D3.1: Report on ab initio band structure calculations and symmetry/topology analyses in antiferromagnets

This report summarizes the work of the ASPIN project consortium on ab initio band structure calculations and symmetry/topology analyses in antiferromagnets. It spans a broad range of works from the study of the topological metal-insulator transition in Dirac semimetal antiferromagnets, to anomalous Hall effect in Weyl semimetal antiferromagnets. Apart from references to our comprehensive reviews, covering our as well as world-wide research in the field, the report outlines our original results in selected specific topics. We give references to the corresponding publications featuring details of these results and for each topic we also explicitly list the contributing teams from the consortium comprising: Institute of Physics in Prague (IOP), University of Nottingham (NOT), Max-Planck Institutes (MPG), IGS Ltd. (IGS), Charles University in Prague (CHU), Johannes Gutenberg University in Mainz (JGU).

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1 Reviews

1.1 Topological antiferromagnetic spintronics

Contributing teams: JGU, IOP, NOT

The recent demonstrations of electrical manipulation and detection of antiferromagnetic spins have opened up a new chapter in the story of spintronics. In this work [1], we review the emerging research field that is exploring the links between antiferromagnetic spintronics and topological structures in real and momentum space. Active topics include proposals to realize Majorana fermions in antiferromagnetic topological superconductors, to control topological protection and Dirac points by manipulating antiferromagnetic order parameters, and to exploit the anomalous and topological Hall effects of zero-net-moment antiferromagnets. We explain the basic concepts behind these proposals, and discuss potential applications of topological antiferromagnetic spintronics.

1.2 Symmetry and Topology in Antiferromagnetic Spintronics

Contributing teams: JGU, IOP, NOT

Antiferromagnetic spintronics focuses on investigating and using antiferromagnets as active elements in spintronics structures. Last decade advances in relativistic spintronics led to the discovery of the staggered, current-induced field in antiferromagnets. The corresponding Néel spin-orbit torque allowed for efficient electrical switching of antiferromagnetic moments and, in combination with electrical readout, for the demonstration of experimental antiferromagnetic memory devices. In parallel, the anomalous Hall effect was predicted and subsequently observed in antiferromagnets. A new field of spintronics based on antiferromagnets has emerged. In this review [2] we focus on the introduction into the most significant discoveries which shaped the field together with a more recent spin-off focusing on combining antiferromagnetic spintronics with topological effects, such as antiferromagnetic topological semimetals and insulators, and the interplay of antiferromagnetism, topology, and superconductivity in heterostructures (see Fig. 1).

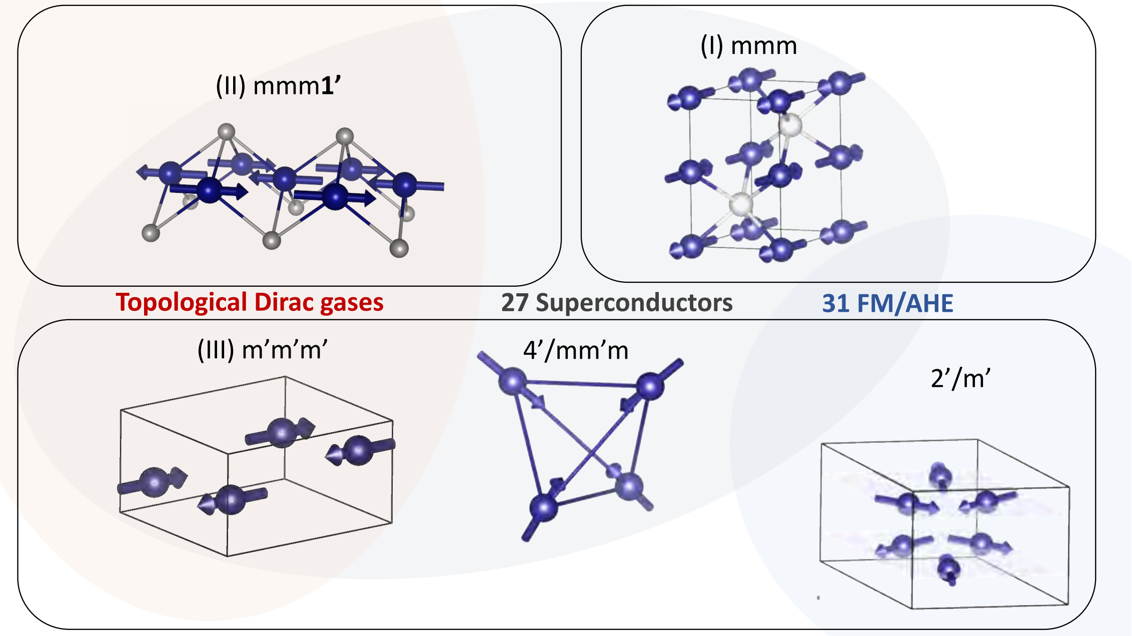

Figure 1: Classical magnetic point groups and exemplar antiferromagnets; the three colors represent overlap of the antiferromagnetic symmetries allowing for Dirac quasiparticles, superconductivity, and anomalous Hall effect [2].

1.3 Route towards Dirac and Weyl antiferromagnetic spintronics

Contributing teams: JGU, IOP, NOT

Topological quantum matter and spintronics research have been developed to a large extent independently. In this review [3], we discuss a new role that the antiferromagnetic order has taken in combining topological matter and spintronics. This occurs due to the complex microscopic symmetries present in antiferromagnets that allow for, e.g., topological relativistic quasiparticles and the newly discovered Néel spin-orbit torques to coexist. We first introduce the concepts of topological semimetals and spin?orbitronics. Secondly, we explain the antiferromagnetic symmetries on a minimal Dirac semimetal model and the guiding role of ab initio calculations in predictions of examples of Dirac and Weyl antiferromagnets: SrMnBi2, CuMnAs, and Mn3Ge. Lastly, we illustrate the interplay of Dirac quasiparticles, topology and antiferromagnetism on: (i) the experimentally observed quantum Hall effect in EuMnBi2; (ii) the large anomalous Hall effect in Mn3Ge; and (iii) the theoretically predicted topological metal-insulator transition in CuMnAs.

2 Dirac an Weyl band crossings in antiferromagnets

2.1 Topological metal-insulator transition and anisotropic magnetoresistance in Dirac semimetal CuMnAs

Contributing teams: JGU, IOP, NOT

In this work [4] we identify a nonsymmorphic crystal symmetry protection of Dirac band crossings in CuMnAs whose on and off switching is mediated by the Néel vector reorientation. We predict that this concept, verified by minimal model and density functional calculations in the CuMnAs semimetal antiferromagnet, can lead to a topological metal-insulator transition driven by the Néel vector reorientation and to the corresponding topological anisotropic magnetoresistance (see Fig. 2).

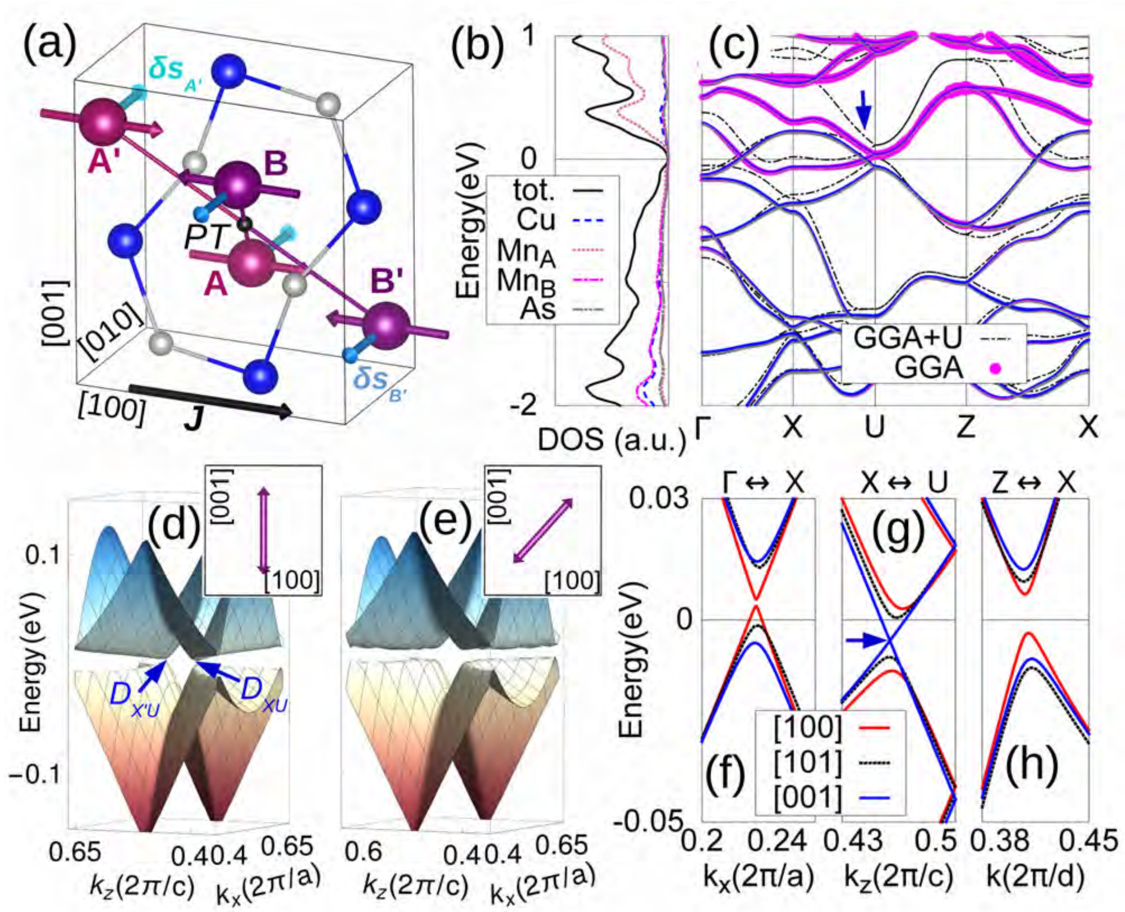

Figure 2: Ab initio study of the topological metal-insulator transition controlled be the Néel vector reorientation in a Dirac semimetal orthorhombic CuMnAs [4].

2.2 Ab initio study of spectral function and resistivity anisotropy in Mn2Au

Contributing teams: JGU, IOP, CHU, NOT

In this work [5] we have elucidated the origin of the large anisotropic magnetoresostance observed in antiferromagnetic Mn2Au by performing ab initio transport calculations and by inspecting anisotropies in the spectral function (see Fig. 3). A large contribution to the anisotropic magnetoresostance originates form opening and closing of a Dirac point near the Fermi level, as predicted in our above earlier theory work [4].

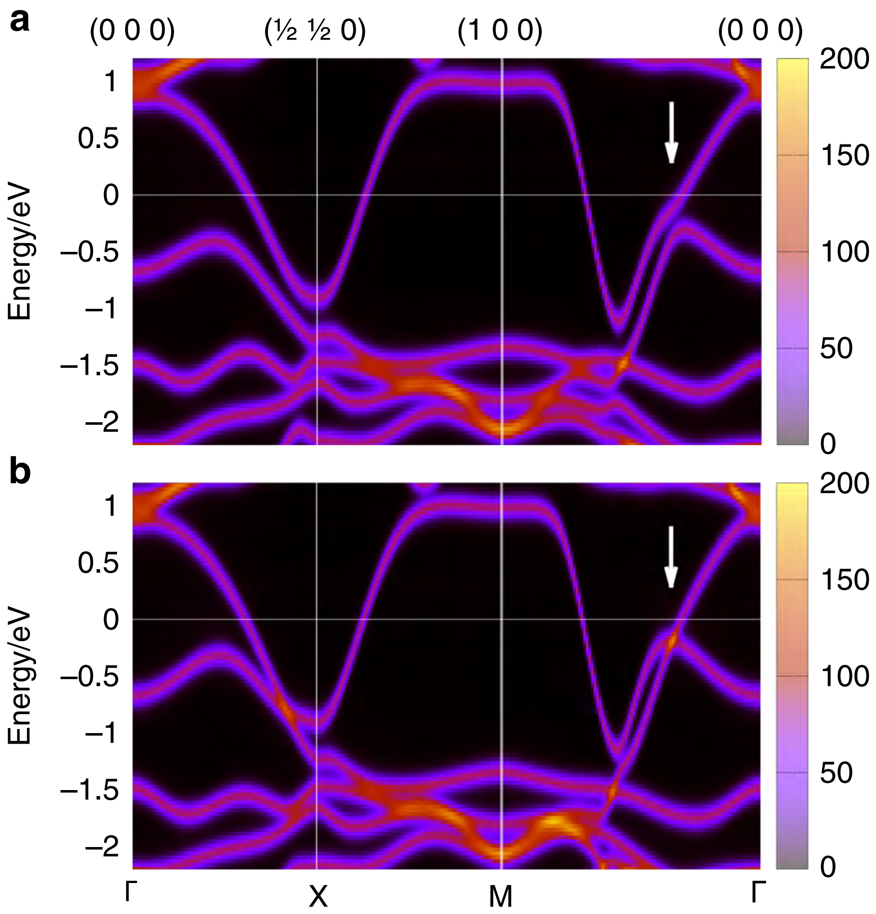

Figure 3: Bloch spectral function calculated in Mn2Au for two orthogonal orientations of the Néel vector; changes near the Dirac crossing are highlighted by arrows [5].

2.3 Magnetic Weyl semimetal without spin-orbit coupling and strong anomalous Hall effect in Ti2MnAl

Contributing team: MPG

In this work [6] we predict a magnetic Weyl semimetal in the inverse Heusler Ti2MnAl (see Fig. 4), a compensated ferrimagnet with a vanishing net magnetic moment and a Curie temperature of over 650 K. Despite the vanishing net magnetic moment, we calculate a large intrinsic anomalous Hall effect (AHE) of about 300 S/cm. It derives from the Berry curvature distribution of the Weyl points, which are only 14 meV away from the Fermi level and isolated from trivial bands. Different from antiferromagnets Mn3X (X = Ge, Sn, Ga, Ir, Rh, and Pt), where the AHE originates from the non-collinear magnetic structure, the AHE in Ti2MnAl stems directly from the Weyl points and is topologically protected. The large anomalous Hall conductivity (AHC) together with a low charge carrier concentration should give rise to a large anomalous Hall angle. In contrast to the Co-based ferromagnetic Heusler compounds, the Weyl nodes in Ti2MnAl do not derive from nodal lines due to the lack of mirror symmetries in the inverse Heusler structure. Since the magnetic structure breaks spin-rotation symmetry, the Weyl nodes are stable without spin-orbit coupling. Moreover, because of the large separation between Weyl points of opposite topological charge, the Fermi arcs extent up to 75% of the reciprocal lattice vectors in length. This makes Ti2MnAl an excellent candidate for the comprehensive study of magnetic Weyl semimetals. It is the first example of a material with Weyl points and large anomalous Hall effect despite a vanishing net magnetic moment.

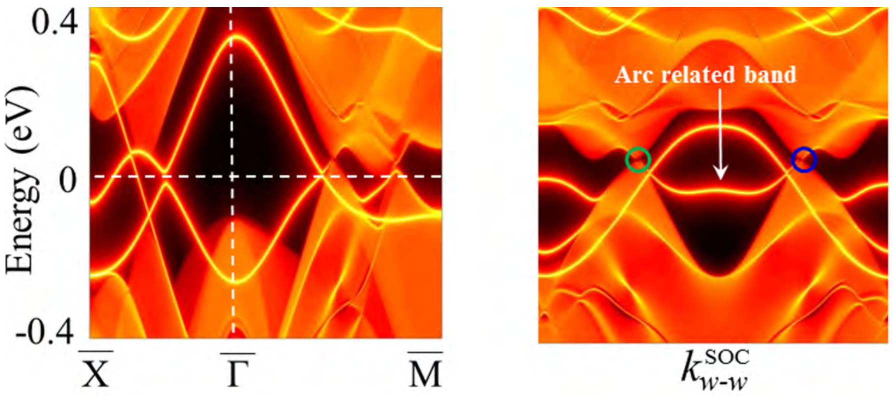

Figure 4: Surface energy dispersion of Ti2MnAl along high symmetry lines and crossing one pair of Weyl points [6].

3 Band structure of CuMnAs probed by ab initio calculations and optical and photoemission spectroscopy

Contributing teams: CHU, IOP, JGU, NOT

The tetragonal phase of CuMnAs progressively appears as one of the key materials for antiferromagnetic spintronics due to efficient current-induced spin-torques whose existence can be directly inferred from crystal symmetry. Theoretical understanding of spintronic phenomena in this material, however, relies on the detailed knowledge of electronic structure which has so far been tested only to a limited extent. In this work [8] we show that AC permittivity (obtained from ellipsometry) and UV photoelectron spectra agree with density functional calculations. Together with the x-ray diffraction and precession electron diffraction tomography, our analysis confirms recent theoretical claim that copper atoms occupy lattice positions in the basal plane of the tetragonal unit cell.

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