ACCEPTED MANUSCRIPT

Editorial

To cite this article before publication: Philip Hofmann *et al* 2021 *Electron. Struct.* in press https://doi.org/10.1088/2516-1075/abf1cb

Manuscript version: Accepted Manuscript

Accepted Manuscript is "the version of the article accepted for publication including all changes made as a result of the peer review process, and which may also include the addition to the article by IOP Publishing of a header, an article ID, a cover sheet and/or an 'Accepted Manuscript' watermark, but excluding any other editing, typesetting or other changes made by IOP Publishing and/or its licensors"

This Accepted Manuscript is **© 2021 IOP Publishing Ltd**.

During the embargo period (the 12 month period from the publication of the Version of Record of this article), the Accepted Manuscript is fully protected by copyright and cannot be reused or reposted elsewhere.
As the Version of Record of this article is going to be / has been published on a subscription basis, this Accepted Manuscript is available for reuse under a CC BY-NC-ND 3.0 licence after the 12 month embargo period.

After the embargo period, everyone is permitted to use copy and redistribute this article for non-commercial purposes only, provided that they adhere to all the terms of the licence https://creativecommons.org/licences/by-nc-nd/3.0

Although reasonable endeavours have been taken to obtain all necessary permissions from third parties to include their copyrighted content within this article, their full citation and copyright line may not be present in this Accepted Manuscript version. Before using any content from this article, please refer to the Version of Record on IOPscience once published for full citation and copyright details, as permissions will likely be required. All third party content is fully copyright protected, unless specifically stated otherwise in the figure caption in the Version of Record.

View the article online for updates and enhancements.

This content was downloaded from IP address 31.51.215.151 on 25/03/2021 at 09:40

Editorial

Philip Hofmann[1,*] and Phil D. C. King[2,†]

[1]*Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark*

[2]*SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, UK*

(Dated: March 18, 2021)

Solid state physicists have long classified the electronic bands of crystals according to their irreducible representations within the relevant space group. However, the concept of *topology* was first introduced into electronic structure theory in the 1980s in connection with the quantum Hall effect. While arguments could be made to explain the extreme precision of the quantised conductance [1], topological considerations provide a much deeper understanding of the conditions leading to the existence of protected edge states [2].

More than a decade ago, the family of quantum Hall effects was extended by the quantum spin Hall effect [3, 4], arsing from topological considerations in connection with the band structure of specific solids. In the first realisation of the quantum spin Hall effect, one-dimensional transport was realised on the edges of a HgTe quantum well with a thickness that was specifically designed to achieve a topological inversion in the band gap of the material. Soon after, it was shown that metallic surface states on certain insulators can be protected by the bulk band topology, leading to a three-dimensional version of the quantum spin Hall effect, the so-called topological insulator [5]. Materials with this property included well-known thermoelectrics such as Bi_2Se_3 and Bi_2Te_3. Similar to the situation of the quantum Hall effect, the idea that the bulk band structure could enforce the existence of certain type of electronic surface states was not new [6], and even properties such as the protection of surface state electrons against back-scattering had been demonstrated [7] – but the derivation of these ideas from topological principles *was* new and lead to the discovery of many other "topological" materials, such as topological semimetals, nodal-line semimetals and materials realising quasiparticle versions of Dirac and Weyl fermions.

The electronic structures of topological materials are fascinating for a number of reasons. From a fundamental point of view, they emphasise the possibility of realising hitherto elusive particles proposed in high-energy physics, for example the Majorana or Weyl fermions – as quasiparticles in a solid. From a purely practical perspective, the Dirac cone-type electronic structure often encountered in topological materials raises hopes to exploit the materials in novel energy-saving electronic devices. Graphene, the simplest material showing a Dirac cone dispersion feeds this hope because of the ultra-high carrier mobility that can be achieved due to an electronic structure with a helical (pseudo)-spin structure, a vanishing phase space for scattering at charge neutrality and, critically for practical applications, a very high Debye temperature (unfortunately, this is not typically found in other topological materials which often contain heavy atoms to boost the spin-orbit coupling strength). High carrier mobilities are indeed found in many topological semimetals, at least at low temperature. Moreover, some of these materials show a huge and non-saturating magnetoresistance with possible applications in magnetic sensing.

While transport properties are of central practical importance for topological materials, it is extremely challenging to infer the topological nature of the electronic structure from transport experiments alone, except for the strictly one-dimensional quantum spin Hall or quantum anomalous Hall effects that are characterised by a quantised edge conductance. Transport signatures of metallic surface states on topological insulators are already much harder to find for several reasons: (1) the band gap of the materials can be small, leading to a large number of intrinsically excited carriers; (2) the materials have a tendency to be degenerately doped and therefore essentially metallic – also in the bulk; (3) the topological surface states are protected against back-scattering, but there is a finite probability for scattering in any other direction, resulting only in a small increase in mobility as compared to a spin-degenerate two-dimensional electron gas; (4) the interesting topological states might be realised in (projected) band gaps far away from the Fermi energy and therefore not accessible to transport experiments. An illustration of these situations is shown in Fig. 2 in Ref. [8] in this Focus Issue.

A key experimental technique for the identification and study of topological electronic states has therefore been angle-resolved photoemission spectroscopy (ARPES), often with additional spin resolution (SARPES). This technique offers access to the detailed $E(k)$ dispersions of occupied electronic states in the solid. In this way, it can be used to observe not only topological states at the Fermi level but also those at higher binding energies. Its momentum resolution provides an immediate route to distinguish between what is often a multitude of topologically trivial and non-trivial states, while its surface sensitivity makes it uniquely suited to study topological surface states. The capabilities of (S)ARPES are ideally matched to theoretical predictions of topological surface band structures that are either full calculations

Accepted Manuscript

or merely based on an inspection of the bulk topological invariants, leading to testable predictions of the basic surface state dispersion topology such as the number of Fermi contours encircling a high symmetry point. Moreover, the spin information obtained from SARPES can reveal predicted properties such as a helical spin textures. Finally, ARPES is able to experimentally distinguish between two-dimensional surface states and three-dimensional bulk states, as well as to search for specific three-dimensional bulk features, such as Dirac or Weyl points. As such, it has proved instrumental in the study of topological materials in recent years.

This Focus Issue of Electronic Structure assembles a collection of articles which, while quite small, provide an excellent overview of the state-of-the-art in ARPES from topological materials.

The review by J. Hugo Dil [8] is focused on SARPES of topological materials. It summarises the technical capabilities and limitations of spin determination in ARPES and how the approach relates to ARPES experiments exploiting circular dichroism. The technical introduction is followed by a summary of the most important contributions form SARPES for different types of topological materials such as topological insulators and semimetals. The discussion of the results is matched with an accessible description of the physics leading to a particular spin texture.

The contribution by P. K. Das *et al.* discusses transport and band structure properties of the transition metal dichalcongenide (TMD) WTe_2 [9]. This material has been named as a candidate for hosting type-II Weyl fermions but, as the paper points out, these quasiparticles are expected to be found above the Fermi level and it is not currently possible to draw a firm conclusions on their realisation in WTe_2 based on the observed surface states alone. Nevertheless, WTe_2 shows intriguing transport properties often associated with topological materials, in particular an extremely large and non-saturating magnetoresistance that can be ascribed to the perfect balance between tiny electron and hole pockets at the Fermi level. The material could therefore find important applications in the detection of magnetic fields.

The paper by O. J. Clark and coworkers discusses a long overlooked and intuitive mechanism for generating topologically protected states that result from the different $k_\perp$ dispersions of p orbital-derived states along high-symmetry directions of the Brillouin zone, leading to topological surface states and bulk band crossings that are protected by crystalline symmetries. The principles are illustrated using calculations and ARPES data from TMDs, emphasising that the strength of the spin-orbit coupling is not crucial for the creation of the topologically protected states. The paper concludes with a discussion of the idea's generality and gives several other examples of topologically protected states that can be explained using the proposed framework. The use of (S)ARPES is particularly important in this work because many of the predicted states exist far from the Fermi energy.

The Focus Issue is concluded by an original research paper by S. Roth *et al.* which discusses the synthesis of a two-dimensional nodal line semimetal (Cu_2Si) such that it is encapsulated between the substate it is grown on and a protective layer of graphene. Interestingly, the material retains its promising electronic properties in this configuration.

After more than ten years of intense research, the bulk band structure topology in the single-particle picture, the resulting topological surface states and their detection with (S)AREPES now comprise a rather mature field. So mature, in fact, that J. Hugo Dil points out that "just because something can be classified by topology does not necessarily render it interesting" [8].

Still, there are still many open questions and poorly understood aspects of band structure topology. Examples are the interplay of topology with magnetism or other kinds of (non-equilibrium) symmetry breaking, such as the presence of transport currents [10]. Also, most of the currently explored materials can be well-described in a single-particle picture and the interplay of band topology and strong correlations needs to be explored. Finally, a particularly interesting aspect of topological band structures arises upon transient band structure engineering by ultrashort light pulses, leading to fascinating situations that are yet to be probed by ARPES, such as the so-called Floquet topological insulator in graphene [11].

* Electronic address: philip@phys.au.dk
† Electronic address: pdk6@st-andrews.ac.uk

[1] R. B. Laughlin, Phys. Rev. B **23**, 5632 (1981).
[2] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).
[3] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science **314**, 1757 (2006).
[4] M. Konig, S. Wiedmann, C. Brune, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science **318**, 766 (2007).
[5] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[6] J. B. Pendry and S. J. Gurman, Surface Science **49**, 87 (1975).
[7] J. I. Pascual, G. Bihlmayer, Y. M. Koroteev, H. P. Rust, G. Ceballos, M. Hansmann, K. Horn, E. V. Chulkov, S. Blugel, P. M. Echenique, et al., Physical Review Letters **93**, 196802 (2004).
[8] J. H. Dil, Electronic Structure **1**, 023001 (2019).
[9] P. K. Das, D. D. Sante, F. Cilento, C. Bigi, D. Kopic, D. Soranzio, A. Sterzi, J. A. Krieger, I. Vobornik, J. Fujii, et al., Electronic Structure **1**, 014003 (2019).
[10] A. C. Balram, K. Flensberg, J. Paaske, and M. S. Rudner, Physical Review Letters **123**, 246803 (2019).
[11] T. Oka and H. Aoki, Phys. Rev. B **79**, 081406 (2009).

Accepted Manuscript