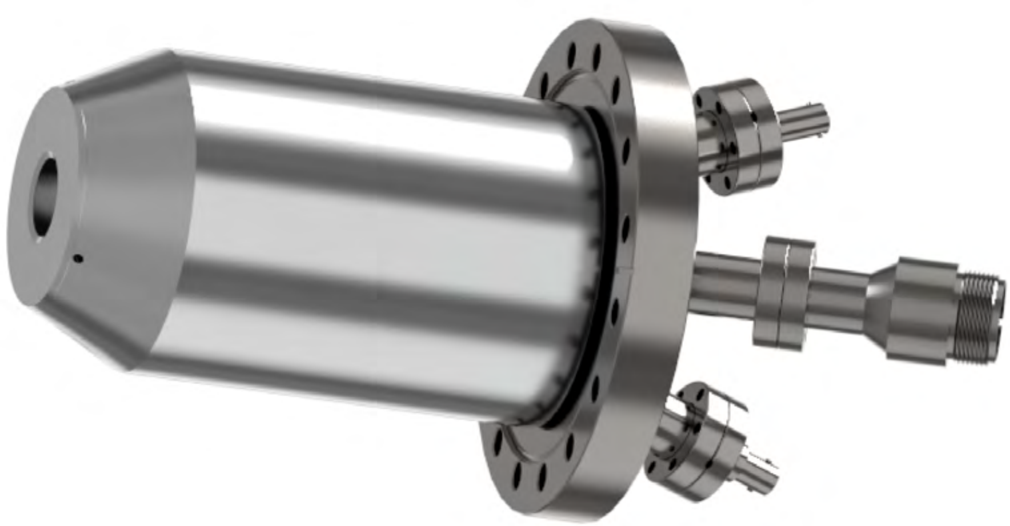
# Elite electrons

Sergey Borisenko, Alexander Fedorov, Andrii Kuibarov, Saicharan Aswartham, Sabine Wurmehl, Bernd Büchner

Die elektronische Struktur spielt eine immer bedeutendere Rolle bei der Entwicklung neuartiger Quantenmaterialien. Die experimentelle Bestimmung dieser elektronischen Struktur war bisher sehr aufwändig und erfordert immer noch erhebliche Ressourcen. Das IFW Dresden hat eine neuartige Technologie entwickelt und patentiert, die es ermöglicht, die wichtigsten Eigenschaften des Elektronenverhaltens mit einem Bruchteil der verwendeten Zeit und Kosten im Vergleich zu den herkömmlichen Techniken zu ermitteln. Die Technologie wurde in einem Prototyp-Spektrometer implementiert. Derzeit vertreibt das IFW-Spin-off-Unternehmen *Fermiologics* erfolgreich eine kommerzielle Version des Geräts.

Electronic structure plays an increasingly important role in the development of novel quantum materials. Until now, the experimental determination of the electronic structure has been very laborious and still requires considerable resources. IFW Dresden has patented a novel technology that allows the determination of the most important properties of the electron behavior with a fraction of the time and cost compared to conventional techniques. The technology has been implemented in a prototype spectrometer, and currently an IFW spin-off company *Fermiologics* is successfully marketing a commercial version of the device.

Abb. 1: FeSuMa® 1.0 Elektronenspektrometer hergestellt von Fermiologics im IFW Dresden. Die 200-mm-Version dieses Geräts würde auf diese Seite passen. Dieses einfache und kompakte Design ist ein bedeutender Fortschritt gegenüber herkömmlichen halbkugelförmigen Analysatoren. *Bild: Fermiologics*
Fig. 1: FeSuMa® 1.0 electron spectrometer produced by Fermiologics in IFW Dresden. 200mm version of this device would fit on this page. This simple and compact design is a significant advance over conventional hemispherical analyzers. *Image: Fermiologics*



Everything that surrounds us depends on the movement of electrons. This motion holds atoms together and makes the existence of materials possible. The energy of only about 3 milligrams of electrons is sufficient to propel Tesla Roadster hundreds of kilometers over a period of hours [1]. This is because only a fraction of all electrons, namely those with the highest energies, determine most of the physical properties of a material, such as the ability to conduct electric current, reflect light, generate electromagnetic waves, magnetism, plasticity, and so on. Knowing exactly how these elite electrons behave would help us to better understand existing materials, improve them and design new ones.
One cannot describe the motion of every single electron, but it seems that the ones we are interested in just want a certain momentum in each direction. In theory, each metal at absolute zero temperature can be uniquely characterized by a Fermi surface - locus of endpoints of exactly such momenta vectors brought to the common origin. It is this, essentially three-dimensional construct, a kind of ID of the material, which is sufficient to derive many of its physical properties.

Angle-resolved photoemission spectroscopy (ARPES) is in principle capable of determining Fermi momenta, but so far only small parts of the 3D Fermi surfaces have been explored experimentally in detail. The main reason for this is that the experimental apparatus is still quite sophisticated and determining a single Fermi vector with high precision takes a relatively long time. Our new methodology is precisely designed to measure the 3D Fermi surfaces and allows the 2D slices of them to be seen live on the PC screen. A high-resolution 3D mapping can then be performed within tens of minutes. Surprisingly, the most technologically complicated element of our experimental setup has been known since the sixties of the last century.

Humanity has been aware of electric charges for a long time, but the first trajectories of electrons, were observed and photographed by Wilson in his famous cloud chamber just over a hundred years ago [2]. Well, those were the electrons emitted spontaneously from a radioactive material, but how can one learn about electrons inside stable matter? This year is the anniversary of Einstein being awarded the Nobel Prize in Physics for explaining the photoelectric effect - a great scientific discovery whose importance can hardly be overestimated. It also provided the answer to our question - electrons can be ejected from the sample by ultraviolet light! Moreover, measuring the energies and momenta of such photoelectrons, one can derive the corresponding values inside the material by using the fundamental conservation laws. In particular, those photoelectrons, having the largest kinetic energies are our elite electrons.

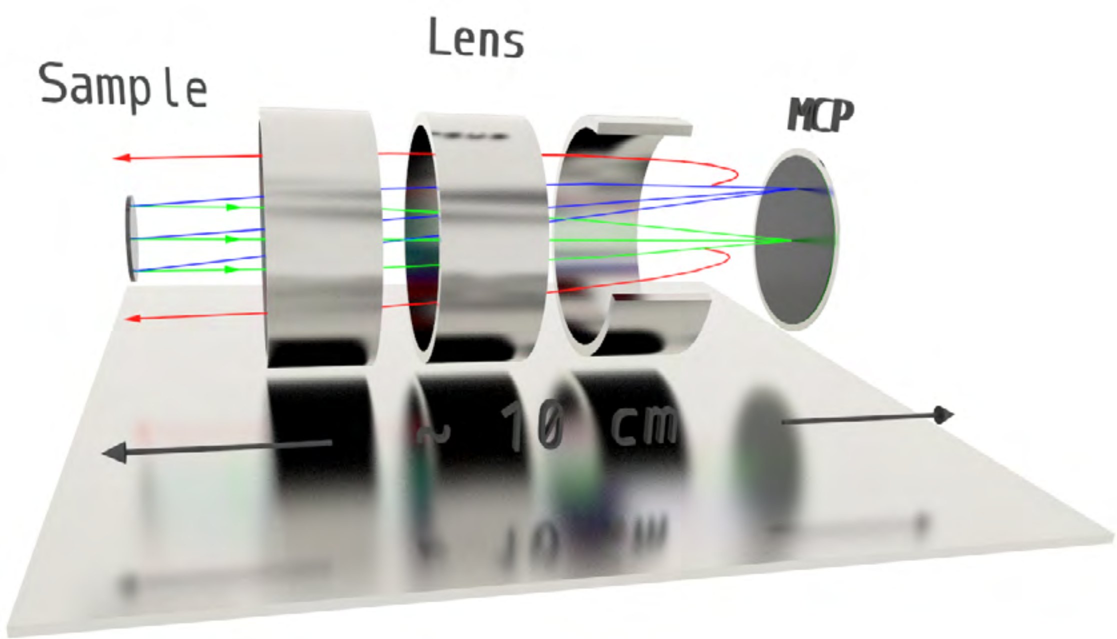
It is the direction of the ejected photoelectrons, which became better visible in subsequent photographs published by Wilson [3], that attracted the attention of Arthur Compton. Although the author himself remarked that “The cathode rays appear to start in all directions…” [3], Compton noticed that electrons are emitted at a certain angle [4]. This event can be seen as the birth of ARPES, as later Compton and others became directly interested in the angular distribution of photoelectrons using Wilson’s chamber and made groundbreaking contributions to the field. It is therefore not a surprise that both gentlemen shared Nobel Prize in 1927.

Cloud chambers were used to study electron trajectories until the 1930s, when the first channel multipliers based on secondary electrons were invented [5]. From then on, even a single electron could be detected because it produced an avalanche of secondary electrons, resulting in a noticeable current spike that can be picked up by common equipment. It was then realized that the performance of such multipliers is not a function of the channel length or the channel diameter separately, but only a function of their ratio [6]. Thus, almost an arbitrary reduction of size is possible. The first operational microchannel plate (MCP), an array of millions of miniature electron multipliers oriented parallel to one another, has been built in the beginning of sixties [7].
MCPs, being able to detect a two-dimensional distribution of photoelectrons, are intensely used in different types of ARPES analyzers until today. However, in order to determine 3D Fermi surface,

one needs to select photoelectrons having highest kinetic energy and count them in all directions. The directions corresponding to the local maxima in the angular distribution would be our sought-after Fermi momenta. This procedure has to be then repeated for a range of photon energies, since a single hν allows probing only a sphere of particular radius in the momentum space. The smaller the step with which the photon energies are sampled, the denser the coverage of the momentum space with concentric spheres of different radius. In other words, one has to record photocurrent as a function of four variables - photon energy, kinetic energy and two angles defining the direction. But MCP allows to count electrons as a function of only two of them.

Nowadays, among the many different types of electron analyzers, the hemispherical ones have become the most popular. Their nontrivial schematic drawings even became associated with the term "ARPES", which you can easily check by typing these letters into your browser. However, this approach is based on the parallel detection of only one of the angles and kinetic energy, i.e. MCP records intensity distribution as a function of angle and kinetic energy, thus probing only a narrow stripe in momentum space. Sampling another dimension in angular space requires many more measurements and leads to an anisotropic angular resolution, let alone full 3D mapping. There are other methods that use pulsed radiation and/or gratings as energy filters, but their efficiency with respect to measurements of 3D Fermi surfaces is even lower. As a consequence, only 2D Fermi surface maps or interpolations are available in the literature and our knowledge about the essentially three-dimensional ID of a given material remains strongly limited.
Recently, we proposed a novel technique [8] that simplifies the whole process and makes 3D Fermi surfaces easily accessible with high resolution. We use an electronic lens that focuses all photoelectrons that have left the surface at a certain angle to a single point directly on MCP, as shown in the Figure 1 with green and blue beams. In this way, we capture a more intuitive for angle-resolved photoemission two-dimensional angular distribution of intensity at once. The key novelty here is that we use the same MCP to select kinetic energies. Since we are only interested in the electrons with the largest kinetic energies, the only task is to filter out the electrons with lower kinetic energies. This is done simply by applying a negative retarding potential to the MCP

Abb. 2: Einfache ARPES. Die Methode ist schematisch dargestellt. Die Elektronen stammen von der Probenoberfläche. Die grünen Strahlen entsprechen der normalen Emission. Blaue Strahlen stellen Elektronen dar, die in einem Winkel von 10° in der vertikalen Ebene emittiert werden. Die roten Strahlen sind die Elektronen mit niedrigerer kinetischer Energie aus beiden Strahlen, die durch das Bremsfeld abgelenkt werden. Drei Zylinder stellen die Elektronenlinse dar. MCP ist der positionsempfindliche Detektor.
Fig. 2: Simple ARPES. Schematics of the method is shown. Electrons originate at the sample surface. Green rays correspond to normal emission. Blue rays represent electrons emitted at 10° angle in the vertical plane. Red rays are the electrons having lower kinetic energies from both beams, deflected by the retarding field. Three cylinders represent the electron lens. MCP is the position-sensitive detector.



front. The result is that the slower electrons (red beams in the Figure 1) do not reach the detector and we get a live image of a 2D section of the Fermi surface on the MCP. One can now successively take such images by varying the photon energies and plot only local maxima as a function of all three momentum components [9]. An example of such a dataset is shown in Figure 2 - this is the first truly high-resolution 3D Fermi surface map of $TiTe_2$ [10]. Electric vehicles, smartphones and skyscrapers are mostly made of metallic materials, each with a unique Fermi surface. Quantum technologies, including computing, are convincingly entering our everyday lives and require novel quantum materials that can be created through electronic structure design. We hope that similar to the progress in the transition from photography to cinematography, our technique will make material architecture in momentum space realistic.

Acknowledgement
SVB is grateful to BMWi for the support within the *WIPANO* project. The work is supported by BMBF via *UKRATOP* program.

References
[1] https://www.tesla.com/blog/weighty-matters-involving-electrons
[2] C T R Wilson, Proc R Sot London, Ser A, 85, 285-288 (1911)
[3] C T R Wilson, Proc R Sot London, Ser A, 87, 277-292 (1912)
[4] A H Compton, Bull Nat1 Res Count (US ), 4, 1-56 (1922)
[5] P. T. Farnsworth, Electron Multiplier, U.S. Patent N. 1, 969, 399 (1930)
[6] J. L. Wiza, Nucl. Instrum. Methods 162, 587-601 (1979)
[7] W. C. Wiley and C. F. Hendee, IRE Trans. Nucl. Sci. NS-9, 103 (1962)
[8] Patent: S. Borisenko, DE102017130072, US11133166B2
[9] This interactive animation visualizes the method in more details: https://webdemo.3dit.de/ifw/detektor/
[10] S. Borisenko et al. preprint arXiv:2105.15055

Cooperations
Fermiologics, Dresden, Germany
Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Denmark
Kyiv Academic University, Ukraine
Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Germany
Max Planck Institute for Solid State Research, Germany
Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland

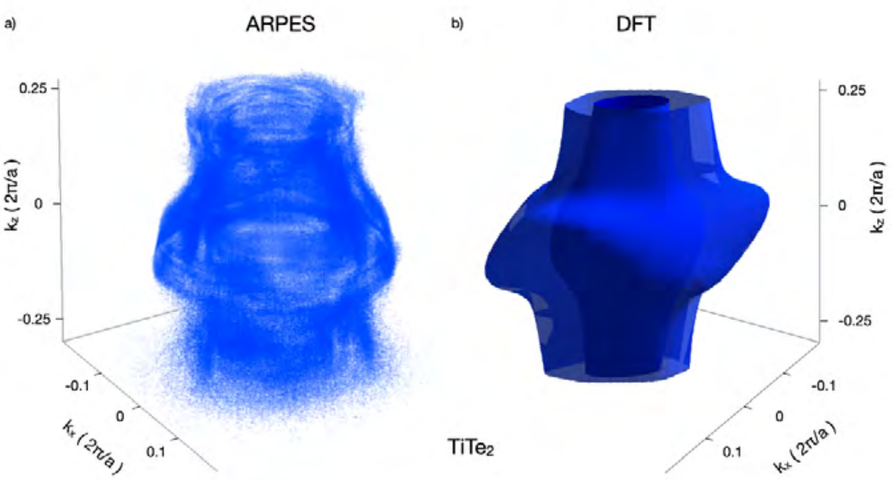



Abb. 3: Dreidimensionale Fermi-Fläche von $TiTe_2$ a) Ein Voxelgramm der Photoemissionsintensität, aufgenommen mit dem FeSuMa-Analysator und Synchrotronlicht. Photonenenergien zwischen 14 und 34 eV werden in 0,2 eV-Schritten abgetastet. Dargestellt sind Voxel innerhalb des normalisierten Intensitätsintervalls zwischen 0,012 und 0,020. Die Gesamtzahl der Punkte des zugrunde liegenden Datensatzes beträgt 1,71924e+07. Die durchschnittliche Intensität liegt bei 0,007, das absolute Maximum bei 0,041. b) Berechnete Fermi-Fläche von $TiTe_2$ im gleichen Impulsvolumen.

Fig. 3: Three-dimensional Fermi surface of $TiTe_2$ a) A voxelgram of photoemission intensity recorded using FeSuMa analyzer and synchrotron light. Photon energies between 14 and 34 eV are scanned with 0.2 eV step. Voxels within normalized intensity interval between 0.012 and 0.020 are shown. Total number of points of the underlying dataset is 1.71924e+07. Average intensity is 0.007, absolute maximum is 0.041. b) Calculated Fermi surface of $TiTe_2$ within the same momentum volume.