Ubiquitous formation of bulk Dirac cones and topological surface states from a single orbital manifold in transition-metal dichalcogenides

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Transition-metal dichalcogenides (TMDs) are renowned for their rich and varied bulk properties, while their single-layer variants have become one of the most prominent examples of two-dimensional materials beyond graphene. Their disparate ground states largely depend on transition metal d-electron-derived electronic states, on which the vast majority of attention has been concentrated to date. Here, we focus on the chalcogen-derived states. From density-functional theory calculations together with spin- and angle-resolved photoemission, we find that these generically host a coexistence of type-I and type-II three-dimensional bulk Dirac fermions as well as ladders of topological surface states and surface resonances. We demonstrate how these naturally arise within a single p-orbital manifold as a general consequence of a trigonal crystal field, and as such can be expected across a large number of compounds. Already, we demonstrate their existence in six separate TMDs, opening routes to tune, and ultimately exploit, their topological physics.

The classification of electronic structures based on their topological properties has opened powerful routes for understanding solid state materials. The now-familiar $\mathbb{Z}_2$ topological insulators are most renowned for their spin-polarised Dirac surface states residing in inverted bulk band gaps. In systems with rotational invariance, a band inversion on the rotation axis can generate protected Dirac cones with a point-like Fermi surface of the bulk electronic structure. If either inversion or time-reversal symmetry is broken, a bulk Dirac point can split into a pair of spin-polarised Weyl points. Unlike for elementary particles, Lorentz-violating Weyl fermions can also exist in the solid state, manifested as a tilting of the Weyl cone. If this tilt is sufficiently large, so-called type-II Weyl points can occur, now formed at the touching of open electron and hole pockets.

Realising such phases in solid-state materials not only offers unique environments and opportunities for studying the fundamental properties of fermions, but also holds potential for applications exploiting their exotic surface excitations and bulk electric and thermal transport properties. Consequently, there is an intense current effort focused on identifying compounds which host the requisite band inversions. In many cases, however, this
depends sensitively on fine details of a material’s electronic or crystal structure. This is partly because almost all known topologically non-trivial phases are stabilised by inversions between states derived predominantly from different atomic manifolds in two- (or more) component compounds (e.g., Bi and Se $p$ orbitals in Bi$_2$Se$_3$ [28] Bi $p$ and Na $s$ orbitals in Na$_3$Bi [2] Nb $d$ and P $p$ orbitals in NbH$_2$[29]). In contrast, here we uncover a simple and remarkably-robust mechanism for realising a hierarchy of band inversions within a single orbital manifold. Across the broad family of 2H- and 1T-structured transition-metal dichalcogenides (TMDs) [20][32], we observe and classify how this mediates the formation of strongly-tilted type-I and type-II bulk Dirac cones as well as ladders of topological surface states (TSSs) and topological surface resonances.

**Band inversions from a single orbital manifold**

Figure 1 details the general principle underlying our findings. As a minimal model, we consider a 2-site system with space group $C_{3v}$, with $3 \times 2$ $p$ orbitals per site in a trigonal crystal field. Such an arrangement naturally describes, for example, the chalcogen layers of the 1T-TMDs (Fig. 1(a)). Fig. 1(c) summarises the splitting of the $p$-orbital energy levels as a result of bonding, crystal field splitting, and spin-orbit coupling. The bands that form from these will in general be anisotropic as the out-of-plane $p_z$ orbitals will have much larger hopping along the out-of-plane direction than the in-plane $p_x/y$ orbitals. For simplicity, we therefore initially neglect inter-layer hopping of the in-plane orbitals, leading to dispersionless $E$- ($p_x/y$)-derived levels as a function of the out-of-plane momentum, $k_z$. The $A_1$ ($p_z$-derived) bands, however, retain a strong $k_z$-dispersion (Fig. 1(d)). When the bandwidth arising due to inter-layer hopping becomes larger than the crystal field splitting (CFS), the $A_1$-derived band will cross through the $E$-derived ones, creating a set of $k_z$-dependent band inversions solely within the $p$-orbital derived manifold of states. In general, anti-crossing gaps can open at these intersections. This is indeed what should occur at the crossings of $R^\perp$ with $R^\parallel$ bands (Fig. 1(e)), as they both share the same symmetry character and angular momentum $m_J = 1/2$. They have opposite parity, however, and thus their hybridization leads to an inverted band gap with a $Z_2$ topological order. Accordingly, these gaps can be expected to host topological surface states, as we demonstrate below.

In contrast, the $R^\parallel$ and $R^\perp$-derived bands belong to different irreducible representations. As a result, they behave differently under the application of the rotational operator $C_{3v}$ (see Supplementary Fig. S1), and their crossing is protected against hybridization as long as it occurs at a $k$-point with $C_{3v}$ symmetry and the host system has both inversion and time-reversal symmetries [37][38]. For the model considered here, this is satisfied for all $k$-points along the $\Gamma$-$A$ direction of the three-dimensional Brillouin zone ($k_x = k_y = 0$, varying $k_z$, see Fig. 1(b)). Consequently, the crossing of the $R^\perp$ and $R^\parallel$-derived bands will lead to a single point of degeneracy (i.e., a bulk Dirac point) located part-way along this direction.
Its location in momentum space is set both by the bandwidth of the $R^+_{1\delta}$-derived band and by the strength of the CFS.

In the schematic shown here (Fig. 1(e)), one branch of the Dirac cone is highly dispersive along $k_z$ while the other is completely dispersionless. This would place such Dirac cones exactly on the boundary of a maximally-tilted ‘conventional’ (i.e. type-I) Dirac cone and an over-tilted one (i.e. a type-II bulk Dirac cone, in analogy to the recent classification of type-II Weyl fermions). In reality, the $R^+_{1\delta}$-derived band will still have a finite, if small, out-of-plane dispersion. The group velocity of this band will determine whether a strongly tilted type-I or type-II Dirac cone is obtained.

**Bulk Dirac points and topological surface states in PdTe$_2$**

We show in Fig. 2 that this simple model can be realised surprisingly well in the electronic structure of the TMD superconductor 1T-PdTe$_2$ (space group: $P3m1$). The bands near the Fermi level are almost exclusively $T_e$-derived (see also Supplementary Fig. S1). Along $\Gamma$-$A$ (Fig. 2(a)), two pairs of predominantly $\text{Te} p_{x,y}$ bands are evident within the energy region $E - E_F \sim -1$ to $\sim 2$ eV (red colouring in Fig. 2(a)), which we assign as the crystal-field and spin-orbit split bonding and antibonding $E$ bands in analogy with Fig. 1. They have modest out-of-plane dispersion, although much more significant dispersion can be observed along the in-plane directions consistent with their in-plane orbital character. In contrast, the $p_z$- ($A_1$)-derived states (cyan colouring in Fig. 2(a)) have a dispersion along $\Gamma$-$A$ that spans nearly the entire valence band bandwidth, and thus crosses through the $E$ states as a function of $k_z$.

Above the Fermi level, where the $R^+_{1\delta}$ band intersects the anti-bonding $R^-_{5,6}$ and $R^-_{4\delta}$ states, a clear type-I protected crossing (upper) and an avoided crossing (lower) are formed, respectively. A similar phenomenology is observed for the bands immediately below $E_F$: the first crossing of the $p_z$-derived band with the bonding $R^-_{5,6}$ states leads to another protected BDP, this time of type-II character (see also Supplementary Fig S2). The second crossing is again gapped. In fact, the proximity of this final crossing to both the anti-bonding and bonding-like branches of the $p_z$-derived bands causes an additional inverted gap to open directly below this. The deeper one ($E - E_F \sim -1.7$ eV in Fig. 2(a,b)) is generated directly by the anti-crossing of bonding $R^+_{1\delta}$ and $R^-_{1\delta}$ states, evident from a small kink structure near the $\Lambda$-point of the $R^+_1$ band. The shallower band gap ($E - E_F \sim -1.1$ eV in Fig. 2(a,b)) results from the crossing of bonding $R^+_1$ with both anti-bonding $R_4$ and bonding $R_4$ states. As the latter two states have opposite parities the total parity of the lower band at the $\Lambda$-point becomes opposite to that at the $\Gamma$-point (see Supplementary Fig. S1 for an explicit calculation of band parities), and hence this is also an inverted band gap with $Z_2$ topological order.

These features are well reproduced by our photon energy-dependent angle-resolved-photoemission (ARPES) measurements of the occupied electronic structure (Fig. 2(b)). While the measured spectral features are broadened due to the finite $k_z$-resolution of photoemission, a significant $k_z$ dispersion of a number of states along $\Gamma$-$A$ can still be observed. In the vicinity of $E_F$, we observe a light and more massive band which cross leading to an enhanced spectral weight at a binding energy of $\sim 0.65$ eV close to the bulk $A$-point along $k_z$. The in-plane dispersion of these same states (insets of Fig. 2(c) and Fig. 3(c) and Supplementary Fig. S3) reveal diffuse “filled-in” intensity (again due to finite $k_z$-resolution) forming the upper part of this Dirac cone. Together, these observations and calculations therefore firmly identify the presence of type-II Dirac cones in PdTe$_2$, arising due to the protected crossing of Te $p_{z}$- and $p_{x,y}$-crystal field-split states as they disperse differently with out-of-plane momentum. We note that spectroscopic signatures of the bulk Dirac cone extend up to the Fermi level and hence these Dirac fermions may carry signatures in transport measurements.

Additional states which are non-dispersive in $k_z$, and thus two-dimensional, are also evident in Fig. 2(b). Most prominent is a band visible at $E - E_F \sim -1.7$ eV, an energy at which no bulk states are present along $\Gamma$-$A$. We thus assign this as a surface state. Its in-plane dispersion (Fig. 2(c) and Supplementary Fig. S4) shows a clear Dirac-like dispersion in the vicinity of $\Gamma$, and is well reproduced by our supercell calculations of the surface electronic structure (Fig. 2(d) and Supplementary Fig. S5, see Methods), confirming its surface-derived origin. This has recently been observed by Yan et al. and assigned as a topological surface state. Our measurements and calculations fully support this assignment: we find that it is located within the $k_z$-projected band gap that arises from the lower of the two avoided crossings below the Fermi level, between the $R^+_{1\delta}$ and $R^-_{1\delta}$ bands identified above. To definitively identify its topological nature, we perform additional spin-resolved ARPES measurements (Fig. 2(e) and Supplementary Fig. S6). These reveal that this state is strongly spin-polarised (from fits to energy distribution curves (EDCs), we find an in-plane spin polarisation of $92 \pm 14\%$ ($73 \pm 16\%$) for the upper (lower) branch of this surface state). The spin lies almost entirely within the surface plane and is locked perpendicular to the in-plane momentum, thus exhibiting the helical spin texture that is a defining characteristic of surface states of topological insulators, as also found from our supercell calculations (Supplementary Fig. S4(c)). We refer below to this topological surface state as TSS2.

More subtly, our supercell calculations also reveal an additional surface-localised state forming another two-dimensional Dirac cone-like feature located at the energy of the band gap opened by the crossing of the $R^-_{1\delta}$ and $R^-_{4\delta}$ features.
bands. Unlike for TSS2, however, the band gap in the bulk spectrum opened by this avoided crossing does not span the entire Brillouin zone in $k_z$. The spectral weight of the surface-derived feature therefore lies within the manifold of projected bulk states which disperse around this avoided crossing. It is therefore better defined as a surface resonance rather than a true surface state. Consistent with this, we find that its wavefunction is more dominant on the surface than for TSS2 (Supplementary Fig. S7). Nonetheless, clear signatures of its in-plane spin-polarisation with the same sign as the upper branch of TSS1 (labeled SS in Fig. 2(e,f); see also Supplementary Fig. S6 which shows that this develops some out-of-plane spin canting along $\Gamma - K$). Spin-polarised Fermi arc surface states intersecting the Dirac point would naturally be expected for, e.g., the (100) surface, where the bulk Dirac points project to different surface momenta (see Supplementary Fig. S7). For the experimental (001) cleavage plane, however, the two bulk Dirac points project exactly on top of each other and so such surface Fermi arcs would not naively be expected. Nonetheless, we note that topological surface states pinned to the Dirac point have recently been reported in calculations for other type-II bulk Dirac systems[39].

Ubiquitous formation of BDPs and TSSs

We show in Fig. 3 and Supplementary Fig. S8 how such band inversions can be found in multiple other TMDs with different local and global crystalline sym-
Fig. 3. Generic observation of bulk Dirac fermions and topological surface states in TMDs. (a) Orbitally-resolved out-of-plane bulk electronic structure of (top to bottom) PdTe$_2$, PtSe$_2$, and WSe$_2$, revealing the formation of bulk Dirac points (BDPs) and inverted band gaps (IBGs) as discussed in the text. (b) Surface-projected supercell calculations (along Γ−K), (c) ARPES measurements (top to bottom: $h\nu = 27$ eV, $p$-pol; $h\nu = 64$ eV, $p$-pol, $h\nu = 49$ eV, CR+CL polarisation) and (d) corresponding curvature analysis$^{40}$ show the surface-projected electronic structure of each compound, revealing the presence of the bulk Dirac cones as well as topological surface states located within the IBGs. The insets in (c) show the ARPES data measured with a different photon energy (PdTe$_2$, $h\nu = 24$ eV) or shown with a different colour contrast (PtSe$_2$ and WSe$_2$) to better highlight some key features of the data.

The symmetry, and which exhibit widely varying bulk properties. We first consider the closely-related compound, 1T-PtSe$_2$. This is semi-metallic, with a smaller overlap of chalcogen-derived bonding and anti-bonding states than in PdTe$_2$. The transition metal states again contribute relatively little near to the Fermi level, while the $p_z$-derived chalcogen band can be clearly resolved cutting through the $p_{x,y}$-derived states in the vicinity of $E_F$ (Fig. 3(a)). A single type-II bulk Dirac cone and a pair of TSSs are stabilised in the occupied electronic structure just as for PdTe$_2$. These are evident in our supercell calculations (Fig. 3(b)) and well matched by our experimental ARPES measurements (Fig. 3(c,d) and Supplementary Fig. S9). The spin-orbit coupling of the Se manifold is weaker than that of Te, evident from both the smaller splitting between $E_F$-like states and from smaller anti-crossing gaps which open in the vicinity of unprotected band crossings. The local band gaps in which the TSSs reside are therefore smaller than in PdTe$_2$, causing the upper branches of the TSSs to rapidly “turn over”
to maintain the surface-bulk connectivity as required by their topological origin.

Nonetheless, in contrast to the common picture for well-known topological insulators such as Bi$_2$Se$_3$, the band inversions leading to such topological surface states, as well as the bulk Dirac cone formation, naturally survive this reduction in spin-orbit coupling strength. Indeed, the relevant energy scales for stabilising the topological surface states here are the $p_z$-derived bandwidth vs. the trigonal crystal field splitting. While increased spin-orbit coupling strength will open larger hybridisation gaps, our findings (see Fig. 3(c,d)) demonstrate how the topological surface states survive as topological surface resonances even in the limit where the hybridisation gap opened is significantly smaller than the dispersion of bulk electronic states around this. They should therefore be a very robust feature of the intrinsic $p$-orbital band inversions found here. The recent observation of a type-II BDP in PtTe$_2$ can also be understood within the same classification that we present here, establishing our findings as generic to the group-10 TMD metals and semimetals. We further show in Supplementary Fig. S7 and Supplementary Fig. S8(a,b) how such bulk band crossings/inversions also occur for the high-temperature 1T phase of the group-9 TMD IrTe$_2$. In this system, the trigonal symmetry which protects the BDP is lost upon cooling through a structural phase transition, raising prospects to investigate temperature-driven topological phase transitions and mass gap opening of the type-II Dirac fermions.

Fig. 3 shows how similar states are also stabilised for a different TMD polymorph: the 2H structure of WSe$_2$ (space group: $P6_3/mmc$). Our bulk band structure calculations along $k_z$ (Fig. 3(a)), which are in good agreement with previous photon energy-dependent ARPES measurements reveal a strongly dispersive band with significant $p_z$ orbital character. This is intersected by very weakly dispersing bands at around 1.5 and 1.9 eV (2.7 and 2.9 eV) below the valence band top which we attribute as the anti-bonding (bonding) $E$-like bands, respectively. Unlike for PdTe$_2$, the Fermi level lies in a band gap of both the transition-metal (formally in a $d^2$ configuration) and chalcogen-derived states, and so this system is a semiconductor. Moreover, transition-metal and chalcogen-derived states are no longer well separated in energy, and so the $E$-like bands have a strong transition-metal $d$-orbital character intermixed with their Se $p_{x,y}$ character. The more localised nature of the $d$ vs. $p$ orbitals, together with an increased inter-layer separation, leads to a significantly smaller out-of-plane dispersion of these $E$-like bands than for PdTe$_2$. Finally, the unit cell contains two MX$_2$ (M=transition metal, X=chalcogen) layers in the 2H structure, as compared to a single layer in the 1T structure. This results in an effective backfolding of the bands about the Brillouin zone boundary along $k_z$, doubling each of the $R_{5,6}^2$ bands as seen in our calculations.

The C$_{3v}$-symmetry enforced degeneracy of the $R_4$-$R_{5,6}$ crossings discussed above, however, still holds. Now, therefore, the crossing of the dispersive $R_4$ band with each of the back-folded $R_{5,6}$ bands leads to a pair of closely-spaced bulk Dirac cones. These are almost maximally tilted and, unlike for PdTe$_2$, now additionally host significant transition-metal character at the BDP. Intriguingly, as the back-folding by definition changes the sign of the band’s group velocity, this leads to stacked Dirac points of opposite character (type-II and type-I for the upper and lower crossings, respectively). We observe clear spectral signatures of the in-plane dispersion of these Dirac cones (Fig. 3(c)), but are unable to resolve a splitting of the two cones experimentally due to their small energy separation and strong three-dimensional dispersions. Both crossings of the $R_4$ and back-folded $R_4$ bands become gapped, and would therefore be expected to host topological surface states/resonances as in PtTe$_2$. One such band gap is too small to resolve experimentally, while for the lower branch a clear inverted band gap is opened. Our supercell calculations (Fig. 3(b)) indeed reveal the TSS located within this band gap, spanning between the manifold of bulk states above and below the band gap. Although the resulting band gap is small, the in-plane dispersion is significant. Our ARPES and spin-ARPES measurements (Fig. 3(c) and Supplementary Fig. S10) show clear evidence for the existence of the resulting surface state, its band-gap crossing nature, and its chiral spin polarisation. As shown in Supplementary Fig. S8(c-f), we find similar bulk Dirac cones and inverted band gaps in other 2H-structured TMDs, TaSe$_2$ and NbSe$_2$ (space group: $P6_3/mmc$), despite them hosting a different layer stacking sequence as compared to WSe$_2$. This opens the exciting prospect to investigate the influence of charge order, which these compounds host, and the consequent reconstruction of the electronic structure, on the topological and bulk Dirac states.

Tunability and robustness against inversion symmetry breaking

The principle underlying the formation of bulk Dirac cones and topological surface states here is very general, and can be expected to occur across numerous materials systems. Moreover, our demonstration of their existence across multiple TMDs indicates that there is still significant opportunity to tailor the properties, locations, and nature of these states. To show this explicitly, we construct a tight-binding model for our minimal 2-site system considered in Fig. 1. Fig. 4 shows how varying the inter-layer hopping both within and between neighbouring unit cells, as well as adjusting the ratio of $\sigma$-type and $\pi$-type inter-layer interactions, leads to a rich array of coexisting topological states and phases. Controlling these experimentally should be possible by varying the degree of covalency in the system and tuning the out-
of-plane lattice parameter via atomic substitution or applied uniaxial pressure or strain along the c-axis. Such a strain field would not affect the trigonal symmetry which protects the Dirac points within the inverted phases, but could be used to traverse the phase boundaries, providing powerful routes to tuneable topological phase transitions and the creation or annihilation of bulk Dirac points in TMDs.

Moreover, the insights gained here suggest strategies for the design of Dirac and topological phases. As an illustration of this, we consider replacing one of the Te layers in PdTe$_2$ by Se. In contrast to PdTe$_2$, this structure is non-centrosymmetric. Typically, such a loss of inversion symmetry would be assumed to lift the spin degeneracy, splitting the Dirac point into a pair of Weyl points. In contrast, since the PdTeSe structure we consider retains trigonal symmetry, we find that both spin-degeneracy and the protected Dirac crossing are maintained along the rotational axis (Γ-A), but spin degeneracy is lost elsewhere (Supplementary Fig. S11). The Dirac point in this case can therefore be considered as a protected degeneracy of two Weyl points that would not typically be expected. Our study thus opens routes to the rational design of topological materials, and indicates just how wide a purview topological band structure effects can be expected to have.

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ML, TB, JFu, IV, JR, TKK, and MH maintained the ARPES/SARPES end stations and provided experimental support. KO, MA, and TS synthesised the measured samples. PDCK, OJC, and MSB wrote the manuscript with input and discussion from co-authors. PDCK and MSB were responsible for overall project planning and direction.

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Methods

Calculations: The bulk calculations were performed within density functional theory (DFT) using Perdew-Burke-Ernzerhof exchange-correlation functional as implemented in the WIEN2K program.\textsuperscript{[23]} Relativistic effects including spin-orbit coupling were fully taken into account. For all atoms, the muffin-tin radius $R_{MT}$ was chosen such that its product with the maximum modulus of reciprocal vectors $K_{max}$ become $R_{MT}K_{max} = 7.0$. The Brillouin zone sampling of 1T (2H) structures was carried out using a $20 \times 20 \times 20$ ($20 \times 20 \times 10$) k-mesh. For the surface calculations, a 100 unit tight binding supercell was constructed using maximally localized Wannier functions.\textsuperscript{[23]} The $p$-orbitals of the chalcogen and the $d$-orbitals of the transition metal atoms were chosen as the projection centres.

The phase diagrams and related band structures shown in Fig. [3] were constructed using a 12-band tight-binding model, considering nearest-neighbour $p-p$ hoppings between the chalcogen sites in a trigonal unit cell similar to that of 1T-TMDs, but without any transition metal element. The basis set is accordingly composed of two sites, that of $1T$-TMDs, but without any transition metal element. In-between the chalcogen sites in a trigonal unit cell similar to a model, considering nearest-neighbour hoppings between the chalcogen and the $d$-orbitals of the transition metal atoms.

Quantitative spin-polarisation magnitudes were determined from the relative areas of Lorentzian peak fits to energy distribution curves (EDCs) originating from oppositely magnetised detectors. A Shirley background and Gaussian broadening were included in this analysis.

To determine the PdTe$_2$ $k_z$ dispersion from photon-energy-dependent ARPES, we employed a free electron final state model

$$k_z = \sqrt{\frac{2m}{\hbar^2}(V_0 + E_k \cos^2 \theta)^{1/2}}$$

where $\theta$ is the in-plane emission angle and $V_0$ is the inner potential. We find best agreement to density-functional theory calculations taking an inner potential of 16 eV and a c-axis lattice constant of 5.13 Å.

Data availability statement: The data that underpins the findings of this study are available at http://dx.doi.org/10.17630/27a2dc90-470f-4e69-be1e-5ebbb0f26b739.

ARPES: ARPES measurements of PdTe$_2$ and PtSe$_2$ were performed at the I05 beamline of Diamond Light Source, UK, and most spin-integrated WSe$_2$ measurements at the CASSIOPEE beamline of Synchrotron SOLEIL, France. Additional ARPES measurements of WSe$_2$ were taken at the APE beamline of Elettra Synchrotrone Trieste, Italy, along with the majority of the spin-resolved ARPES measurements. Additional spin-resolved measurements of PdTe$_2$ were obtained from the I3 beamline of MAX IV Laboratory, Sweden.

High-quality single crystal samples, grown by chemical vapour transport, were cleaved in situ at temperatures ranging between 9-15K. Measurements were performed using either $p$-polarised (PdTe$_2$, PtSe$_2$, WSe$_2$), or circularly polarised (WSe$_2$) light, and using photon energies in the range $\hbar \nu = 24 - 132$ eV. Scienta R4000 hemispherical analysers, with a vertical entrance slit and the light incident in the horizontal plane, were used at Diamond and SOLEIL.

A VG-Scienta DA30 analyser (Elettra), fitted with two very low energy electron diffraction (VLEED) based spin polarimeters,\textsuperscript{[27]} was utilised for the majority of the spin-resolved measurements along three momentum directions, while additional measurements were performed using a mini-Mott setup on a Scienta R4000 analyser (Max IV). The finite spin-detection efficiency was corrected using detector-dependent Sherman functions ranging between $S = 0.17 \pm 0.03$ and $S = 0.43 \pm 0.03$ as determined by fitting the spin-polarisation of reference measurements of the Au(111) Rashba-split surface state for each experimental set-up utilised. Spin-resolved EDCs were determined according to

$$I_i^{\pm} = \frac{I_i^0(1 \pm P_i)}{2},$$

where $i = \{x, y, z\}$, $I_i^0 = (I_i^{\uparrow} + I_i^{\downarrow})$ and $I_i^{\pm}$ is the measured intensity for a positively or negatively magnetised detector, corrected by a relative efficiency calibration. The final spin polarisation is defined as follows:

$$P_i = \frac{I_i^{\uparrow} - I_i^{\downarrow}}{S(I_i^{\uparrow} + I_i^{\downarrow})},$$

where $S$ is the relevant Sherman function for the detector in use.

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