Magnetic and defect probes of the SmB\(_6\) surface state

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The impact of non-magnetic and magnetic impurities on topological insulators is a central problem concerning their fundamental physics and possible novel spintronics and quantum computing applications. SmB\(_6\), predicted to be a topological Kondo insulator, is considered a benchmark material. Using a spin-polarized tip in scanning tunneling microscopy destroys the signature peak of the topological surface state, revealing its spin texture. Further, combining local STS with macroscopic transport measurements on SmB\(_6\) containing different substitutions enables us to investigate the effect of impurities. The surface states around impurities are locally suppressed with different length scales depending on their magnetic properties and, for sufficiently high impurity level, globally destroyed. Our study points directly to the topological nature of SmB\(_6\), and unveils, microscopically and macroscopically, how impurities – magnetic or non-magnetic – affect topological surface states.

Topological surface states (TSS) are novel quantum electronic states which not only serve as a playground for realizing many exotic physical phenomena (such as magnetic monopoles, Majorana fermions, and the quantum anomalous Hall effect) but may also find several fascinating applications, e.g. in spintronics or quantum computing.\(^4\) Remarkably, these states are theoretically predicted to be robust against backscattering from non-magnetic impurities due to their chiral spin texture, whereas a magnetic impurity breaks time-reversal symmetry and therefore induces spin scattering. Within the framework of the Anderson impurity model, however, the spin of a magnetic impurity may also be screened by the conduction electrons via the Kondo effect, resulting in an effectively non-magnetic scattering center at sufficiently low temperature.\(^2\) Conversely, nonmagnetic impurities in a Kondo lattice may generate magnetic scattering by locally increasing the density of states or by creating a “Kondo hole” in the lattice. This calls for a detailed understanding of the impact of impurities – non-magnetic and magnetic – on TSS.

SmB\(_6\) was theoretically predicted to be a topological Kondo insulator in which a direct bulk gap is induced by Kondo hybridization, and the TSS reside in this small bulk gap.\(^5\) Compared to weakly correlated topological insulators, SmB\(_6\) features a small, but fully opened bulk gap.\(^5\) Therefore, the TSS dominate the density of states (DOS) at Fermi level \(E_F\) at low temperature, such that insulating bulk and metallic surface properties can be well distinguished in spectroscopic and transport measurements.\(^5\) In addition, the small bulk gap can easily be suppressed by doping, converting the system to a trivial insulator\(^10\). These aspects provide an excellent starting point to study the effects of impurities in SmB\(_6\).

Although the metallic nature of the surface states in SmB\(_6\) has been confirmed by several experiments,\(^9,11–13\) pinning down their topological origin remains challenging and controversial.\(^14–16\) Consequently, detecting the spin-texture of the metallic surface states is cardinal and crucial. Considerable efforts have been made to uncover the helical spin texture of the surface state by spin-resolved ARPES\(^17,18\) and spin injection\(^19\). However, the surface conditions are multifaceted.\(^20\) Therefore, investigations on well defined and non-reconstructed surfaces are important and a microscopic probe is called for. In this respect, scanning tunneling microscopy and spectroscopy (STM/S) studies have clearly demonstrated their ability to characterize the bulk and surface state band of SmB\(_6\).\(^21,22\) In particular, a major contribution to the dominating peak in the low-\(T\) tunneling spectra at a bias voltage \(V_b \approx -6.5\) mV was related to the surface state.\(^23\) Here we employ spin-polarized STS to illustrate the existence of a surface spin texture. The local and global impact of non-magnetic and magnetic impurities on the surface states is further studied by comparing microscopic STS with macroscopic transport measurements.

To investigate the \(-6.5\) mV signature peak of the surface state in more detail, we compare STS spectra obtained by a regular (non-magnetic) W-tip and a magnetic Cr-coated tip (see for tip details) on the same surface of pristine SmB\(_6\). Cr-coated tips are often used for spin-dependent STS measurements.\(^24\) Figure 1 presents the tunneling spectra at 0.35 K on a non-reconstructed surface (see Fig. 2A). At large \(|V_b| > 20\) mV, the spectra measured by the two tips are very similar and featureless indicating that any difference is not due to an exotic DOS of the tip.\(^27\) For small \(|V_b| \lesssim 20\) mV, however, the two d\(I\)/d\(V\)-spectra are markedly different: In the case of the Cr-tip, the pronounced signature peak at \(-6.5\) mV, and hence tunneling into the surface state, is dramatically suppressed\(^25\) and the direct bulk hybridization gap—albeit slightly reduced in size—is exposed.\(^24,26,27\) This is corroborated by
a striking similarity of spectra obtained with magnetic Cr-tip and such recorded with W-tip at 20 K, a temperature at which the surface state has not formed. In addition, as we will show later, scanning with a W-tip over the surface of Gd-substituted SmB$_6$ generates a similar reduction of the $-6.5$ meV peak at low temperatures. In this case, the W-tip may pick up magnetic Gd substituents from the surface, and this process can even be reversed (for details see [23]). Importantly, picking up Gd from the sample converts a regular W-tip into a magnetic tip as, e.g., observed by STM on Fe$_{1+y}$Te where excess Fe atoms were picked up [22]. The close similarity of the spectra obtained with these two types of magnetic tips suggests that the spectral changes are induced by the magnetic nature of the tips, consistent with a spin texture at the surface of SmB$_6$ [23]. However, the reduction in $dI/dV$ upon using magnetic tips, reaching 72% at $V_b = -6.5$ mV is, to the best of our knowledge, extraordinarily large and beyond expectations for spin-polarized STS. Thus, spin-polarized tunneling alone, based on an in-plane alignment of the Dirac electron spins, may not account for this very effective suppression of the signature peak at $-6.5$ meV. This is even more obvious in view of a spin polarization of less than 50% for a Cr-tip [23]. Moreover, a tunneling spectrum obtained at $\mu_0 H = 12$ T is rather similar to zero-field spectra for regular W-tips (Fig. 1), and precludes the possibility of a magnetic stray field of the magnetic tip suppressing the surface state locally.

To scrutinize the effect of magnetism on the surface states of SmB$_6$, we now investigate the local impact of substituents, both non-magnetic (Y) and magnetic (Gd), on these surface states. Figures 2A–C exhibit representative topographies ($8 \times 8$ nm$^2$ field of view) of a pristine, a 3% Y- (SmB$_6$:3%Y) and a 0.5% Gd-substituted sam-

FIG. 1. Tunneling spectra with W and Cr tips. Spectra obtained on non-reconstructed surfaces of pure SmB$_6$ by W-tip (red) and magnetic Cr-tip (blue) at 0.35 K and zero magnetic field ($V_b = 50$ mV, set-point current $I_{sp} = 200$ pA). For comparison, a spectrum taken with a W-tip at a magnetic field of 12 T is presented (pink, vertically offset by 1 nA/V).
FIG. 2. **Influence of impurities on spectroscopic results.** (A)–(C) 8×8 nm² topographies of pure as well as 3% Y- and 0.5% Gd-substituted SmB₆. The cyan arrows indicate the ranges and directions of STS measurements around the impurities. (D)–(F) dI/dV-curves of the three samples measured at 0.35 K and zero field. The curves are measured at positions with increasing distance from the impurity (the impurities are located at #1) along the arrows in (A)–(C), correspondingly (bias voltage $V_b = 30$ mV, current set-point $I_{sp} = 100$ pA). (G)–(I) dI/dV values at $V_b = -6.5$ meV (red) and $-2.5$ meV (blue) with increasing distance from the impurity (impurities are located at 0). The black dashed lines are fits according to the model described in[23]. $h_{sup}$ and $\ell_{sup}$ indicate the suppression of peak intensity at the impurity and its lateral extent, respectively.

is not intended to be applied to non-magnetic impurities we made use of the fact that it describes the experimental data reasonably well to still obtain $h_{sup}$ and $\ell_{sup}$. The apparent applicability of the theoretical model to non-magnetic impurities along with the moderate suppression ($h_{sup} \approx 15\% – 45\%$) may be due to the local changes of the bulk band structure[23,24] and/or the Kondo hole effect[25]. On the other hand, the large magnetic moment of Gd locally breaks time reversal symmetry and may eventually gap out the Dirac cone states. As a result, $h_{sup}^{Gd}$ reaches 70% at the Gd defect, reminiscent of the value obtained by using a Cr-tip. A similar influence of magnetic substituents on the tunneling spectra was also observed in weakly correlated topological insulators, such as Cr-substituted[27,28] or V-substituted[29] Sb₂Te₃.

Our observation of an only local impact of magnetic substituents on the surface state is consistent with an unexpectedly insensitive response of the TSS in Bi₂Se₃ to magnetic impurities at low impurity concentration in a macroscopic measurement[31].

As shown above, the TSS are fully recovered around 2.2 nm from the Gd substituent site. For SmB₆:0.5%Gd, the average distance between Gd substituents is ~2.4 nm. A pressing question at this juncture is: what if the average Gd-Gd distance is reduced to well below $\ell_{sup}$, i.e. if the areas of suppressed surface states sufficiently overlap? To address that, we also probed a SmB₆:3%Gd sample with average Gd-Gd distance of about 1.3 nm. Here, a surface state signature peak was only found in areas where the statistical distribution of Gd atoms resulted in larger...
The resistivity $\rho(T)$ of pure SmB$_6$ exhibits a well-known saturation below around 3 K which is due to surface conductance, see Fig. 3A. A very similar behavior is found for SmB$_6$:3%Y and SmB$_6$:0.5%Gd samples, yet with a much smaller overall change in $\rho(T)$ due to the substituents. For SmB$_6$:3%Gd, the low-$T$ saturation of $\rho(T)$ is indeed not observed, instead $\rho(T)$ continues to increase exponentially, indicating a remaining gap. This is expected when the average Gd-Gd distance is smaller compared to $\ell_{\text{sup}}^{\text{Gd}}$. In highly, non-magnetic substituted SmB$_6$, see example of 18% Y in Fig. 3, the $\rho(T)$-behavior is qualitatively different from non- or lightly substituted samples, possibly due to interacting substituents.

The data presented in Fig. 3B allow an estimate of the changes exerted on the bulk hybridization gap $\Delta$ from $\rho(T) \propto \exp(\Delta/k_B T)$. Pure SmB$_6$ exhibits the typical two gap values$^{32}$ with $\Delta_1 \approx 36$ K for $5 \leq T \leq 12$ K and $\Delta_2 \approx 60$ K for $20 \leq T \leq 40$ K (the latter is marked in Fig. 3B). For the lightly ($\leq 3\%$) substituted samples, somewhat reduced gap values$^{33}$ of $\Delta_1 \approx 24$ K ($9 \leq T \leq 14$ K) and $\Delta_2 \approx 50$ K at higher $T$ are observed, along with an increased surface conductivity, all in line with an substitution-induced modification of the Kondo lattice formation$^{34}$. Yet, these changes in the bulk are minute and apparently too small to account for the dramatic changes in the surface properties. Above $\sim 10$ K, the resistivities are determined by the bulk band structure, and the measured values perfectly overlap for the lightly substituted samples. In contrast, $\rho(T)$ of the highly substituted sample SmB$_6$:18%Y below $\sim 20$ K deviates from exponential behavior.

The resistivity data in Fig. 3 provide compelling support from a global measurement for the local picture obtained from STS (Fig. 2): Around a magnetic substituent, the disturbance is stronger and extends further out compared to non-magnetic impurities. In the former case, the formation of a global conducting surface state in SmB$_6$:3%Gd at low $T$ is already inhibited, providing a microscopic picture of how the topologically protected surface state is destroyed in real space.

Now the pressing question concerns the underlying mechanism for the suppression of the surface state signature peak in STS in both cases, for magnetic tips as well as magnetic substituents in SmB$_6$. The observed disappearance of the peaks at $-6.5$ meV and $-2.5$ meV upon tunneling with magnetic tips or on surfaces of Gd-substituted samples could be either due to a suppression of the actual surface states, or by simply suppressing the tunneling probability into the corresponding states (or a combination thereof). Although we cannot unambiguously distinguish between these two scenarios we consider the similarity of the spectra with suppressed surface state signature peak to those obtained on pristine SmB$_6$ with W-tip at $T = 20$ K, i.e. a temperature at which the surface states have not yet formed, as a strong indication towards the former, i.e. a repressed formation of the surface state, see Fig. S4. The main parameter determining the extent of the suppressed surface state around a magnetic impurity is related to the exchange interaction$^{35}$. Moreover, the surface state suppression by using magnetic tips calls for an interaction whose energy scale is well beyond the Zeeman energy scale associated with a magnetic field of 12 T, Fig. 1. Therefore, we propose an exchange-interaction based proximity effect to be involved when tunneling with a magnetic tip or around a magnetic substituent.

Our findings have two important consequences. First, they provide a microscopic picture of how the surface states are perturbed by impurities. This perturbation takes place locally at the defect site, with an extent $\ell_{\text{sup}}$ that depends on the magnetic properties of the defect. Enhanced values of $\ell_{\text{sup}}$ and, particularly, $h_{\text{sup}}$ at magnetic substituents as observed by our STM experiments were considered a hallmark for TS$^{32}$. Secondly, the very effective suppression of the surface state signature peak at $-6.5$ meV can be exploited in applications. We propose to use SmB$_6$ to detect exchange fields. If a tunnel-
ing tip is made of SmB$_6$ and scanned over a surface to be investigated, the $dI/dV$-response at $V_0 = -6.5$ mV is expected to change significantly around a magnetic surface atom. Based on our investigations by magnetic tips and on magnetic impurities this effect should allow for single spin detection.

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SUPPLEMENTARY MATERIALS

I. Sample preparation

All samples used in this study were grown by the Al-flux method \((9)\). Single crystals were cleaved \textit{in situ} below \(20\) K to expose a (001) surface. For pristine \(\text{SmB}_6\), 6 different single crystals were cleaved and investigated for this study, for \(0.5\) at.% Gd-substituted \(\text{SmB}_6\) and 3 at.% Y-substituted \(\text{SmB}_6\) three single crystals were investigated.

Pristine \(\text{SmB}_6\) sample are difficult to cleave and atomically flat and well resolved surface areas have to be searched for. By introducing substituents into \(\text{SmB}_6\), the cleavage properties change dramatically and atomically flat areas can be found much more easily. However, the vast majority of the surface areas investigated so far was reconstructed (see also Fig. 3 and related discussion). Again, unreconstructed surface areas have to be searched for.

II. Details of Tunneling measurements

STM measurements were conducted in an ultra-high vacuum \((p < 3 \times 10^{-9} \text{ Pa})\) environment and at a temperature \(T = 0.35 \text{ K}\). The tunneling current \(I\) was measured using tungsten tips or Cr-coated tips. Tunneling parameters for topography, if not noted otherwise, were \(V_b = 300 \text{ mV}\) and \(I_{se} = 200 \text{ pA}\). The differential conductance \((dI/dV)\) spectra were acquired by lock-in technique applying a modulation voltage of typically \(V_{mod} = 0.3 \text{ mV}\); if enhanced resolution was strived for, \(V_{mod}\) was reduced to \(0.05 \text{ mV}\). The bias voltage \(V_b\) is applied to the sample. A magnetic field of up to \(12 \text{ T}\) can be applied perpendicular to the scanned sample surface.

III. Scanning Tunneling Spectroscopy using Cr-tips

For spin-polarized scanning tunneling spectroscopy commercially available Cr-coated tips (NaugaNee-dles LLC; \url{http://nauganeedles.com/products-USSTM_W500-Cr}) were used. Such tips are characterized by uncompensated magnetic moments at the Cr tip apex resulting in a spin-polarization (up to 45%) at the Fermi level \((30)\). In addition to STS on \(\text{SmB}_6\) with magnetic tips in zero field, such measurements have also been conducted in magnetic fields. Selected results of one of the field cycles are presented in Fig. 4. Here, the magnetic field (applied perpendicular to the sample surface) was gradually increased up to \(\mu_0 H = 5 \text{ T}\), consecutively ramped back down to zero field and reversed, with spectra taken at constant field values. Clearly, no significant change in the tunneling spectra is observed. The \(dI/dV\)-data perfectly overlap in the low-field regime, i.e. weak-antilocalization (WAL) effects are not visible in our tunneling spectra. At high magnetic fields the zero-bias conductance is slightly reduced. Such a high applied field may influence the magnetization orientation within our magnetic tip which, in turn, can reduce the tunneling current through spin-polarized effects.

Notably, scanning the Cr-tip over substantial surface areas of pristine \(\text{SmB}_6\) alludes towards the lack of any significant local dependencies of the spectra.

IV. Changing tip conditions on Gd-substituted \(\text{SmB}_6\)

In the following we discuss observations on \(0.5\) at.% Gd-substituted \(\text{SmB}_6\), investigated using W-tips. Initially, the STS spectra obtained on surfaces of such samples and away from defects were very similar to those taken on pure \(\text{SmB}_6\). One example is presented in Fig. 5; orange line marked as “virgin” \((\text{SmB}_6:0.5\text{Gd}, \text{for topography see Fig. 2C of the main text})\). In particular, the surface state signature peak at \(V_b \approx -6.5 \text{ mV}\) is well developed at \(T = 1.8 \text{ K}\).

In Fig. 6 we present more examples of topographies obtained on a surface of a 0.5% Gd-substituted \(\text{SmB}_6\) sample. Atomically resolved topographies are difficult to obtain on surfaces of substituted \(\text{SmB}_6\) (specifically for higher substitution levels) as the tips are frequently changing while scanning, likely due to picked-up atoms or clusters. Note that such a susceptibility to picking up atoms from the surface is in line with the fact that the substituted samples cleave much more easily compared to pure \(\text{SmB}_6\). A sudden, individual tip change is shown in the upward scan Fig. 6 and marked by a white arrow. The effective height difference across this step, taken along the white line in Fig. 6 and plotted in

![Graph showing tunneling spectra with Cr-tip in magnetic field](image-url)
FIG. S2. Converting a non-magnetic into a magnetic tip. All Spectra were obtained on the same non-reconstructed surface of 0.5% Gd-substituted SmB$_6$. Virgin W-tips showed the orange spectrum (virgin), but changed after some scanning into the blue one (pick-up), likely due to picked-up Gd atoms. After applying voltage pulses to the tip, the original spectrum could be restored (red, removed). The blue spectrum matches nicely with those obtained with Cr-tips (Fig. 1 of main text, blue spectrum) indicating that the tip is converted into a magnetic one by picking up entities from the sample surface.

Fig. S3B, of about 25 pm is not expected from the crystallographic structure of SmB$_6$, and no downward step is observed at this position in the subsequent down-scan. Hence, we argue that the tip picked up something from the surface at this particular scan line, consistent with a decreasing tip-sample distance. Since the vast majority of the defects seen in the topographies of substituted samples is caused by the substituents it is highly likely that the tip picked up Gd in this case.

After extensive scanning and several changes in topographic height as just described, we sometimes observed topographies like the one presented in Fig. S3C. Apparently, some tips which are modified by picking up some Gd atoms (or Gd-containing clusters) from the sample surface are reasonably stable to produce atomically resolved topographies. The blue line (length of 1 nm) indicates the line along which 101 spectra were taken and averaged to give the blue curve (“pick-up”) of Fig. S2. Clearly, this spectrum is extremely similar to the one obtained with Cr-coated tip, Fig. 1 of the main text. We note that these spectra were intentionally obtained away from any (visible) defect on the surface. Only after applying several voltage pulses (typically of +10 V) to the tip, these adatoms could be removed from the tip. A topography after such a removal of adatoms is presented in Fig. S3D. We note that such severe voltage pulses significantly disturb the sample surface close to the tip and hence, different sample areas were investigated before and after applying voltage pulses to the tip. The thereafter obtained spectrum, red curve in Fig. S2 ("removed") taken along the red line in Fig. S3D, corresponds to the virgin one.

FIG. S3. Topographies obtained with a W-tip on 0.5% Gd-substituted SmB$_6$ showing the changing tip conditions. (A) While scanning the tip often changed suddenly. Here, such an individual tip change is marked by a white arrow (area 8 $\times$ 4 nm$^2$, up-scan). (B) Height profile along the white line in (A). The upward step is likely related to the tip having picked up something from the surface. (C) Topography (10 $\times$ 10 nm$^2$) after extensive scanning on the surface and numerous tip changes as in (A). Blue line indicates a 1 nm line away from defects over which spectra were taken and averaged to yield the blue curve of Fig. S2. (D) Topography (10 $\times$ 10 nm$^2$) after applying several voltages pulses (up to +10 V) to the tip. Red line: line over which spectra were averaged for red curve in Fig. S2. Because of the voltage pulses different areas were scanned.

The spectra obtained with Cr-coated tip and with W-tip after picking up atoms (or clusters) from the surface (blue curve in Fig. S2) exhibit a particularly effective suppression of the surface state signature peak. Along with the above-mentioned fact that Gd was likely picked up, we surmise that the changes in spectra are due to a conversion of the W-tip apex into a magnetic one by picking up Gd while scanning, similar to observations on Fe$_{1+y}$Te (28) by picking up excess Fe. Extensive scanning revealed that such spectra with suppressed surface state signature peak were obtained everywhere on the sample surface, and not just by positioning the tip accidentally on top of a Gd-substituent. The fact that we can reverse this process through cleaning the tip by applying voltage pulses, i.e. turning the W-tip back to a normal (non-magnetic) one, heavily supports this conjecture. We emphasize that such changes to the tip, i.e. picking up atoms or clusters from the surface with the concomitant spin-polarization in the spectra, and recovering the regular spectra after applying voltage pulses to the tip, were conducted repeatedly on several surfaces of samples with different Gd substitution level and with different W-tips, all with consistent results. Such tip changes were not observed on pristine SmB$_6$ (for pure SmB$_6$ more than 30 cleaved surfaces were investigated so far). This indicates that Gd is important for observing these changes in the
FIG. S 4. The surface state signature peak of SmB$_6$ at $V_b = -6.5$ mV can be suppressed by using magnetic tips (Cr-coated or after picking up Gd from the sample surface, green and red curve, respectively) or by using regular W-tips and raising the temperature to 20 K. From the latter, a $dI/dV$ curve at 0.35 K is estimated (violet dash-dotted line) which coincides with the 20 K-data after thermal broadening.

obtained spectra; its magnetic nature provides a reasonable explanation for observing spectra very similar to the ones seen with spin-polarized Cr-tips. Our corresponding results not only support the spin-polarized nature of tunneling with picked-up tips but also the assignment of the defects observed on the surfaces of Gd-substituted samples to Gd impurities.

V. Comparison of spectra with suppressed surface state signature peak

We have presented several ways to suppress the peak in the tunneling spectra at $V_b = -6.5$ mV which signals the surface state in pure SmB$_6$. This peak suppression can be achieved by using a magnetic tip (either Cr-coated or after having picked up Gd by a W-tip from a Gd-substituted sample) or locally around defects. In Fig. S4, we compare such spectra obtained with magnetic tips, to a $dI/dV$-spectrum obtained at 20 K on a pure SmB$_6$ sample (8), blue curve in Fig. S4. At this temperature, the surface states have not yet formed. In order to allow for a comparison of the different temperatures, we estimated a curve at $T = 0.35$ K (dash-dotted curve in Fig. S4) which, thermally broadened to $T = 20$ K, coincides with the spectrum measured at 20 K. At $T = 0.35$ K, all spectra exhibit a similar suppression of the tunneling conductance $dI/dV$ at low $V_b$, thereby exposing the bulk Kondo gap. This comparison indicates that very likely the surface states themselves are suppressed in all cases, rather than the tunneling probability into the surface states.

VII. Analytical solution to the single magnetic impurity

In this section, we will theoretically discuss the LDOS in a model describing the Dirac surface state of a topological insulator coupled to a single magnetic impurity with exchange interaction [Ref. 32, A. Matulis, F. M. Peeters, Quasibound states of quantum dots in single and bilayer graphene. Phys. Rev. B 77, 115423 (2008)]. The model Hamiltonian of such coupling in polar coordinate is given
FIG. S6. Surface of 3% Y-substituted SmB$_6$. Within the area presented (20×20 nm$^2$) about 50 defects can be counted. The atomically resolved surface is likely B-terminated.

by

$$H_0 = \begin{pmatrix}
  M_0 \Theta(r_0 - r) & -iAe^{i\theta}(\frac{\partial}{\partial r} + i\frac{\partial}{\partial \theta}) \\
  -iAe^{-i\theta}(\frac{\partial}{\partial r} - i\frac{\partial}{\partial \theta}) & -M_0 \Theta(r_0 - r)
\end{pmatrix},$$

where $A(=hv_F)$ is the Fermi velocity of the Dirac electrons, $M_0 = J_2S_z$ is the exchange interaction between Dirac electrons and the magnetic impurity, $r_0$ determines the range of the exchange interaction, and $\Theta(r_0 - r)$ is the step function. As we will see below, $r_0$ will determine the suppression range $r_{\text{sup}}$ while $M_0$ will determine the maximal suppression ratio $h_{\text{sup}}$ of LDOS measured in experiments. Due to the rotation symmetry of the above Hamiltonian, the wave function will take the ansatz

$$\Psi(n) = \frac{1}{\sqrt{2\pi}} \left( e^{i\theta}_n \phi_1(r) \right),$$

where $n$ labels the angular momentum and is a good quantum number. Based on this wave function ansatz, the Schrödinger equation can be simplified as

$$\begin{pmatrix}
  M_0 \Theta(r_0 - r) & -iA(\frac{\partial}{\partial r} - \frac{n\pi}{r}) \\
  -iA(\frac{\partial}{\partial r} + \frac{n\pi}{r}) & -M_0 \Theta(r_0 - r)
\end{pmatrix} \begin{pmatrix} \phi_1,n \\ \phi_2,n \end{pmatrix} = E \begin{pmatrix} \phi_1,n \\ \phi_2,n \end{pmatrix}. $$

The resulting equation for $\phi_1$ is given by

$$\frac{d^2}{dr^2}\phi_{1,n}(r) + \frac{1}{r}\frac{d}{dr}\phi_{1,n}(r) + \left(\frac{E^2 - M_0^2}{r^2} - \frac{n^2\pi^2}{r^2}\right)\phi_{1,n}(r) = 0. \quad (1)$$

Here, $E$ denotes the energy difference between the STS bias voltage and the Dirac point.

The equation for $\phi_{1,n}$ takes the general form of (modified) Bessel functions and thus, we can further simplify our solution. When $|E| \geq |M_0|$, our solution ansatz will be

$$\phi_n = \frac{1}{N} \begin{pmatrix} a(M_0 + E)J_n(k_1r) \\ -iAk_1aJ_{n-1}(k_1r) \end{pmatrix} \quad r < r_0,$$

$$\phi_n = \frac{1}{N} \begin{pmatrix} E(bJ_n(k_2r) + cY_n(k_2r)) \\ -iAk_2(bJ_{n-1}(k_2r) + cY_{n-1}(k_2r)) \end{pmatrix} \quad r > r_0,$$

and when $|E| < |M_0|$, 

$$\phi_n = \frac{1}{N} \begin{pmatrix} a(M_0 + E)I_n(k_1r) \\ -iAk_1aI_{n-1}(k_1r) \end{pmatrix} \quad r < r_0,$$

$$\phi_n = \frac{1}{N} \begin{pmatrix} E(bJ_n(k_2r) + cY_n(k_2r)) \\ -iAk_2(bJ_{n-1}(k_2r) + cY_{n-1}(k_2r)) \end{pmatrix} \quad r > r_0,$$

where $N$ is the normalization factor, $k_1 = \sqrt{|E^2 - M_0^2|}/A$, $k_2 = |E|/A$, $J_n$ and $Y_n$ are Bessel functions, and $I_n$ are modified Bessel functions. The corresponding boundary condition at $r = r_0$ is given by

$$a(E + M_0)J_n(k_1r_0) = E(bJ_n(k_2r_0) + cY_n(k_2r_0)),$$

$$ak_1J_{n-1}(k_1r_0) = k_2(bJ_{n-1}(k_2r_0) + cY_{n-1}(k_2r_0)). \quad (2)$$

for $|E| \geq |M_0|$ and

$$a(E + M_0)I_n(k_1r_0) = E(bJ_n(k_2r_0) + cY_n(k_2r_0)),$$

$$ak_1I_{n-1}(k_1r_0) = k_2(bJ_{n-1}(k_2r_0) + cY_{n-1}(k_2r_0)). \quad (3)$$

for $|E| < |M_0|$.

For the large $r$, we generally take a cut-off, labeled by $R$, to prevent the divergence. The asymptotic form of Bessel functions is given by

$$J_n(kr) \sim \sqrt{\frac{2}{\pi kr}} \cos(kr - \frac{n\pi}{2} - \frac{\pi}{4}),$$

$$Y_n(kr) \sim \sqrt{\frac{2}{\pi kr}} \sin(kr - \frac{n\pi}{2} - \frac{\pi}{4}), \quad (4)$$

for a large $r$. The level spacing is given by $\Delta E = A\pi/R$. As $R$ goes to infinity, the energy spectrum becomes continuous. The normalization factor $N$ is determined by the large $r$ behavior. We can consider the integral of $|\phi_{1,n}|^2$ in the region $[R_0, R]$, where $R \to \infty$. We choose the parameter $R_0$ so that the Bessel functions can be well described by their asymptotic forms when $r > R_0$ ($R_0 > r_0$). As a result, the integral of $|\phi_{1,n}|^2$ in the range $[R_0, R]$ is given by

$$4\pi \int_{R_0}^{R} \left| \phi_{1,n}(r) \right|^2 dr = \frac{4\pi}{N^2} \int_{R_0}^{R} \left| bJ_n(k_2r) + cY_n(k_2r) \right|^2 dr +$$

$$\left| bJ_{n-1}(k_2r) + cY_{n-1}(k_2r) \right|^2] \right. \int_{R_0}^{R} \left| \frac{2}{\pi k_2r} E^2 \left( b^2 + c^2 \right) \right. \right.$$  

$$= 8E^2\left( R - R_0 \right) \frac{1}{k_2 N^2} \left( b^2 + c^2 \right). \quad (5)$$

As $R$ approaches infinity, this integral will diverge linearly, thus being dominant over the integral of $|\phi_{1,n}|^2$ in
other range. Thus, the normalization factor is determined by the integral in the range $[R_0,R]$ and can be chosen as \( \frac{1}{N} = \sqrt{\frac{1}{8|E|AR(b^2+c^2)}} \) for a sufficient large $R$ in the numerical calculation. With the obtained wave function, the LDOS is given by

\[
\rho(r,E) = \frac{R}{A\pi} \sum_n |\Psi_n(r)|^2
\]

\[
= \frac{R}{2A\pi} \sum_n [\phi_{1,n}^2 + \phi_{2,n}^2]
\]

\[
= \frac{1}{16\pi^2 A^2|E|(b^2+c^2)} \sum_n a^2[(M_0 + E)^2J_n^2(k_1r) + \ldots |E^2 - M_0^2|J_n^2(k_1r)]
\]

\[
n\quad r < r_0,
\]

or

\[
= \frac{1}{16\pi^2 A^2|E|(b^2+c^2)} \sum_n E^2[bJ_n(k_2r) + cY_n(k_2r)]^2 + \ldots
\]

\[
(bJ_{n-1}(k_2r) + cY_{n-1}(k_2r))^2
\]

\[
n\quad r > r_0.
\]

To calculate the LDOS around a magnetic impurity and at $E$, there are three free parameters in the equation of $\rho(r,E)$, i.e. $M_0$, $A$, and $r_0$. For SmB$_6$, the Dirac cone is estimated to be around $-5$ meV with a Fermi velocity of 1000 m/s to 10000 m/s, depending on the location of the Dirac cone (at $X$-point or $\Gamma$-point). Here we focus on the dominant peak at $-6.5$ mV, so $E \approx -1.5$ meV. Our STM measurements indicate that $r_0 \approx 2.2$ nm for Gd. Consequently, we are left only with $M_0$ and $A$ as free parameters. As shown in Fig. 2I of the main text, this analytical solution can reproduce our experimental data very well, using $A = 3000$ m/s and $M_0 = 1.35$ meV.

As mentioned in the main text, the proposed model was developed for magnetic impurities and as such, is not necessarily expected to be applicable to non-magnetic impurities as well. However, in order to obtain estimates for $\ell_{sup}$ and $h_{sup}$ in a comparable fashion, we also used this model to describe the LDOS around impurities in the pure and Y-substituted SmB$_6$. Taking the same $E$ and $A$ values as for the Gd-case, we obtained $M_0 = 0.7$ meV and 1.35 meV for pure and Y-substituted SmB$_6$, respectively, while $r_0$ has the same value of 1.5 nm in both cases. Also, because of the uncertain applicability of the model in case of non-magnetic impurities we kept a distinction between $r_0$ (the exchange interaction range in the model) and $\ell_{sup}$ (the experimentally observed suppression of the LDOS).