

Supplementary Information for “observation of a spin-textured nematic Kondo lattice”

Theoretical model:

Here we propose a simple phenomenological model to describe nematic hybridization in USbTe. This material has space group $P4/nmm$ and thus D_{4h} tetragonal point group. The STM data reveals tetragonal symmetry breaking along the diagonals on the (a,b) plane. This is consistent with a nematic order with a form factor $k_x k_y$ in momentum space, which transforms as the B_{2g} irreducible representation (irrep) of the point group D_{4h} and lowers the point group to the orthorhombic D_{2h} .

We first use group theory to determine which type of hybridization order parameter $\Delta =$

$\langle \sum_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \text{h.c.} \rangle$ transforms as the B_{2g} irrep. Here, $c_{\mathbf{k}\sigma}$ is the fermionic operator for the itinerant electrons and $f_{\mathbf{k}\sigma}$ refers to the local f -orbitals of the U atom. There are seven different f orbitals, which we label in terms of the usual cubic harmonics f_{z^3} , f_{xz^2} , f_{yz^2} , f_{xyz} , $f_{x(x^2-3y^2)}$, $f_{y(3x^2-y^2)}$, and $f_{z(x^2-y^2)}$. In the presence of the crystal fields of USbTe, they transform as 4 different irreps: A_{2u} , B_{1u} , B_{2u} and E_u , as shown in the Supplementary Tables 1 and 2. As for the itinerant electrons $c_{\mathbf{k}\sigma}$, we can consider either the U d -orbitals or the Sb p -orbitals. In the first case, there are five different orbitals, d_{z^2} , $d_{x^2-y^2}$, d_{xy} , d_{xz} , d_{yz} , which transform as 4 different irreps: A_{1g} , B_{1g} , B_{2g} and E_g (see Supplementary Table 1). In the latter case, there are three different orbitals p_x , p_y , p_z which transform as 2 irreps: A_{2u} and E_u (see Supplementary Table 2).

In Supplementary Tables 1 and 2, we show the symmetry of the hybridization order parameter for all possible combinations between f and d or p orbitals in terms of the irreps of D_{4h} . If we enforce the condition that the hybridization order parameter must be purely nematic and transform as B_{2g} , there are only three options:

$$\Delta = \langle \sum_{\mathbf{k}\sigma} f_{xyz,\mathbf{k}\sigma}^\dagger p_{z,\mathbf{k}\sigma} + \text{h.c.} \rangle \quad (1)$$

$$\Delta = \langle \sum_{\mathbf{k}\sigma} f_{xz^2,\mathbf{k}\sigma}^\dagger p_{y,\mathbf{k}\sigma} + f_{yz^2,\mathbf{k}\sigma}^\dagger p_{x,\mathbf{k}\sigma} + \text{h.c.} \rangle \quad (2)$$

$$\Delta = \langle \sum_{\mathbf{k}\sigma} f_{x(x^2-3y^2),\mathbf{k}\sigma}^\dagger p_{y,\mathbf{k}\sigma} - f_{y(3x^2-y^2),\mathbf{k}\sigma}^\dagger p_{x,\mathbf{k}\sigma} + \text{h.c.} \rangle \quad (3)$$

The fact that none of the combinations involving f - d hybridization gives a pure nematic order parameter is a simple consequence of the fact that the two orbitals have opposite parities. However, if we relax the condition that the order parameter must be a pure B_{2g} nematic, but allow it to break other point-group symmetries besides fourfold rotations, the number of options increases substantially. In this case, Δ transforming as E_u or E_g can also support a secondary composite B_{2g} nematic order parameter. To understand this, we note that because E_u and E_g are two-dimensional irreps, the hybridization gap is a two-component order parameter $\Delta = (\Delta_1, \Delta_2)$. It turns out that we can combine these two components to define a composite order parameter $\varphi = \Delta_1 \Delta_2$ that transforms precisely as the B_{2g} nematic order

parameter. It is important to emphasize that if either an E_u or an E_g type of hybridization order parameter Δ condenses, other symmetries of the tetragonal lattice will be broken besides the fourfold rotational symmetry. In particular, if only fourfold rotations are broken by the hybridization (i.e. Δ transforms as B_{2g}), the resulting point group is the orthorhombic D_{2h} , which possesses inversion and two vertical mirrors. In contrast, if the condensed Δ transforms as E_g , the resulting point group is the monoclinic C_{2h} , which possesses inversion but no vertical mirrors. Finally, if Δ transforms as E_u , its condensation lowers the point group to the orthorhombic C_{2v} , which does not possess inversion although it does have vertical mirrors. Further experiments are needed to unambiguously determine whether the system has vertical mirrors and inversion in the nematic phase.

Having established that only hybridization order parameters of the form Eq (1)-(3) transform as a pure nematic B_{2g} order parameter, we now discuss its fingerprints on the electronic dispersion of the heavy Fermi liquid state by using a standard mean-field description⁶⁰⁻⁶⁴. We start by considering the case of p_z itinerant electrons and f_{xyz} local orbitals, with hybridization given by Eq (1). The mean-field Hamiltonian is given by $H = H_0 + H_{\text{hyb}}$ with:

$$\begin{aligned} H_0 &= \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} p_{\mathbf{k}\sigma}^\dagger p_{\mathbf{k}\sigma} + \tilde{E}_f \sum_{\mathbf{k}} f_{\mathbf{k}\sigma}^\dagger f_{\mathbf{k}\sigma} \\ H_{\text{hyb}} &= \sum_{\mathbf{k}\sigma} \tilde{\Delta}_{\mathbf{k}} (f_{\mathbf{k}\sigma}^\dagger p_{\mathbf{k}\sigma} + p_{\mathbf{k}\sigma}^\dagger f_{\mathbf{k}\sigma}) + \sum_{\mathbf{k}\sigma} \Delta (f_{\mathbf{k}\sigma}^\dagger p_{\mathbf{k}\sigma} + p_{\mathbf{k}\sigma}^\dagger f_{\mathbf{k}\sigma}) \end{aligned} \quad (4)$$

where Δ is the hybridization order parameter given by Eq (1) and $\tilde{\Delta}_{\mathbf{k}} = \tilde{\Delta} \sin k_x \sin k_y$ is the symmetry-preserving hybridization between p and f orbitals. Here, $\varepsilon_{\mathbf{k}}$ is the dispersion of the itinerant electrons and $\tilde{E}_f$ is the renormalized f -electron energy. We would like to emphasize the difference between Δ and $\tilde{\Delta}_{\mathbf{k}}$. The first one is the direct hybridization between p and f orbitals and as such it breaks the tetragonal symmetry of the lattice. Consequently, its onset must be accompanied by a phase transition. As for the second term, $\tilde{\Delta}_{\mathbf{k}}$, it does not break any symmetry of the lattice, and as such it is non-zero at any temperature. In a heavy Fermi liquid description, $\tilde{\Delta}_{\mathbf{k}}$ is expected to show a pronounced enhancement at the Kondo coherence temperature, displaying a crossover behavior rather than a phase transition.

To break the fourfold rotational symmetry, both Δ and $\tilde{\Delta}_{\mathbf{k}}$ must be non-zero. To see this, we can integrate out the f electrons and treat H_{hyb} perturbatively in powers of $\Delta^2/\tilde{E}_f$ we find the following correction to the itinerant electron dispersion:

$$\delta H_0 = \frac{1}{\tilde{E}_f} \sum_{\mathbf{k}\sigma} (\Delta^2 + \tilde{\Delta}^2 \sin^2 k_x \sin^2 k_y + 2\Delta \tilde{\Delta} \sin k_x \sin k_y) p_{\mathbf{k}\sigma}^\dagger p_{\mathbf{k}\sigma} \quad (5)$$

The first two terms preserve tetragonal symmetry, whereas the second one breaks it, as it clearly transforms as the B_{2g} irrep. Therefore, the band dispersion in the heavy Fermi liquid phase, $E_{\pm}(\mathbf{k})$, exhibits nematic features only when $\Delta, \tilde{\Delta} \neq 0$, with:

$$E_{\pm}(\mathbf{k}) = \frac{\varepsilon_{\mathbf{k}} + \tilde{E}_f}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathbf{k}} - \tilde{E}_f}{2}\right)^2 + (\Delta + \tilde{\Delta}_{\mathbf{k}})^2} \quad (7)$$

To illustrate this behavior, we show in Supplementary Fig.7 the dispersion (7) of the heavy Fermi liquid phase along the two diagonals, which are related by a 90° rotation. The red curve corresponds to $\Delta \neq 0$

and $\tilde{\Delta} = 0$, whereas the blue curve corresponds to $\Delta \neq 0$ and $\tilde{\Delta} \neq 0$. Clearly, the fourfold rotational symmetry of the band dispersion is broken in the latter case only.

The same situation happens in the case where the (p_x, p_y) itinerant orbitals hybridize with either $(f_{x(x^2-3y^2)}, f_{y(3x^2-y^2)})$ or (f_{xz^2}, f_{yz^2}) orbitals, corresponding to the hybridization order parameters given by Eqs. (2) and (3). For simplicity of notation, we denote the orbitals as (p_1, p_2) and (f_1, f_2) . The Hamiltonian in this case is given by:

$$H_0 = \sum_{k\sigma} (A_k \tau_0^{ij} + B_k \tau_z^{ij} + C_k \tau_x^{ij}) p_{i,k\sigma}^\dagger p_{j,k\sigma} + E_f \sum_{k\sigma} (f_{1,k\sigma}^\dagger f_{1,k\sigma} + f_{2,k\sigma}^\dagger f_{2,k\sigma})$$

$$H_{\text{hyb}} = \sum_{k\sigma} (\Delta + \tilde{\Delta}_k) (f_{1,k\sigma}^\dagger p_{2,k\sigma} \pm f_{2,k\sigma}^\dagger p_{1,k\sigma} + \text{h. c.})$$

where the plus sign corresponds to the case of (f_{xz^2}, f_{yz^2}) orbitals whereas the minus sign corresponds to the case of $(f_{x(x^2-3y^2)}, f_{y(3x^2-y^2)})$ orbitals. Here, τ_μ are Pauli matrices in p -orbital space. As in the previous case, Δ is the hybridization order parameter given by Eqs. (2) or (3), whereas $\tilde{\Delta}_k = \tilde{\Delta} \sin k_x \sin k_y$ is the symmetry-preserving hybridization. Moreover, the terms

$$A_k = -(t_\sigma + t_\pi)(\cos k_x + \cos k_y) - \mu$$

$$B_k = -(t_\sigma - t_\pi)(\cos k_x - \cos k_y)$$

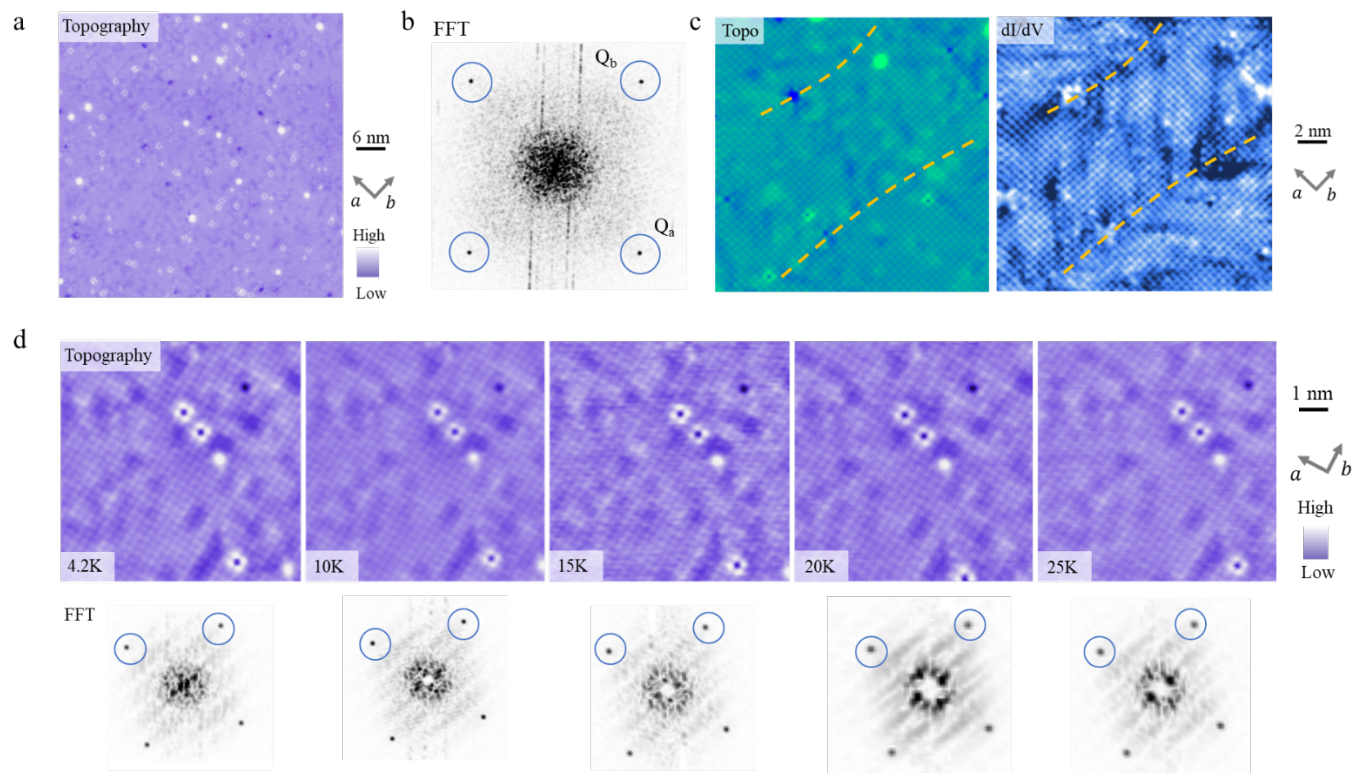
$$C_k = -2t_d \sin k_x \sin k_y$$

correspond to p_x, p_y orbitals with nearest- and next-nearest-neighbor hopping terms on the square lattice. In the limit $t_d = 0$ (nearest-neighbor hopping only), an analytical expression for the four dispersions in the heavy Fermi liquid phase is available:

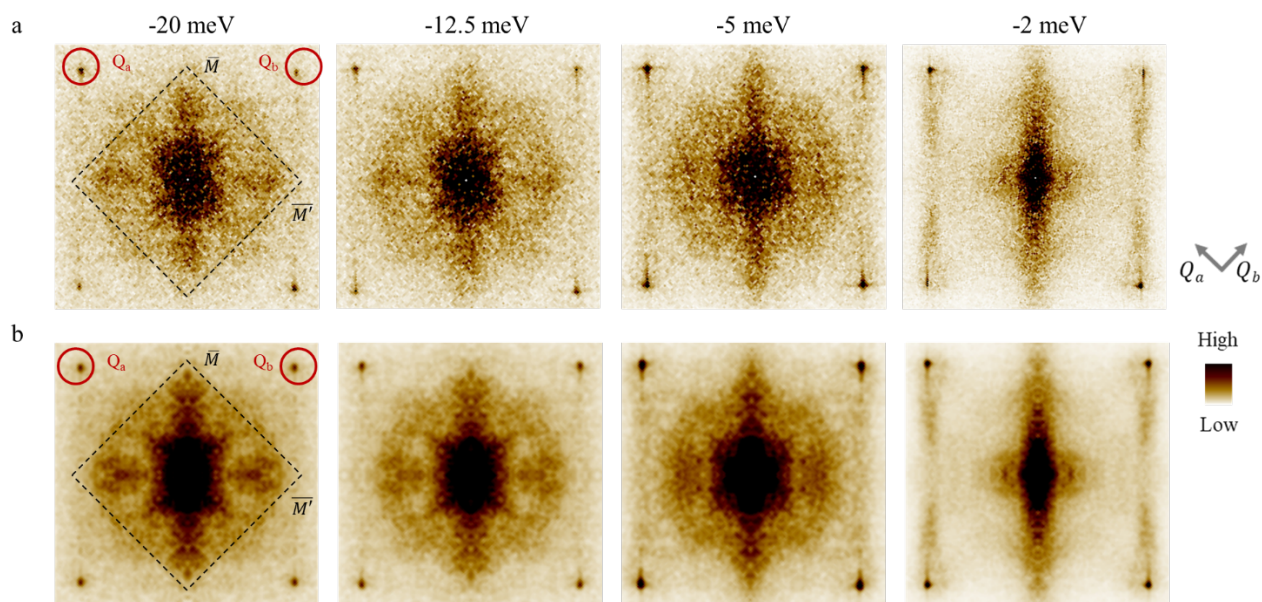
$$E_\pm^\epsilon(\mathbf{k}) = \left(\frac{A_k + \epsilon B_k + \tilde{E}_f}{2} \right) \pm \sqrt{\left(\frac{A_k + \epsilon B_k - \tilde{E}_f}{2} \right)^2 + (\Delta + \tilde{\Delta}_k)^2}$$

with $\epsilon = \pm 1$. The case $t_d \neq 0$ can be solved numerically in a straightforward way. In either case, we find indeed that a nematic distortion of the band dispersion is only present when both $\Delta, \tilde{\Delta} \neq 0$.

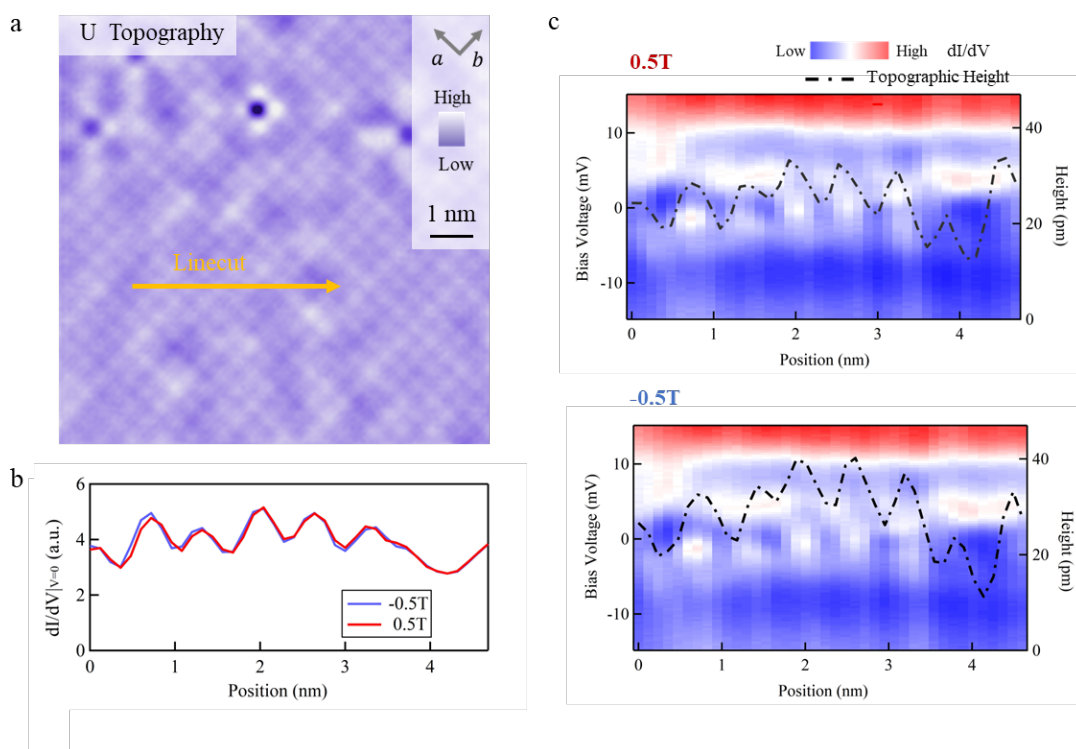
1. C. Lacroix, M. Cyrot, Phase diagram of the Kondo lattice. *Phys. Rev. B*, **20**, 1969 (1979).
2. N. Read, D. Newns, A functional integral approach to the Anderson lattice with f-f hopping. *J. Phys. C*, **16**, L1055 (1983).
3. A. Auerbach, K. Levin, Kondo Bosons and the Kondo Lattice: Microscopic Basis for the Heavy Fermi Liquid. *Phys. Rev. Lett.*, **57**, 877 (1986).
4. A. J. Millis, P. A. Lee, Large-orbital-degeneracy expansion for the lattice Anderson model. *Phys. Rev. B*, **35**, 3394 (1987).
5. P. Coleman, Mixed valence as an almost broken symmetry. *Phys. Rev. B*, **35**, 5072 (1987).



Supplementary Figure 1. Demonstration of no lattice reconstruction and structure disorder. **a**, Large-area topography on U termination at 4.2K. **b**, Fourier-transform of topographic image. Bragg peaks are circled. Bragg peak intensity is homogeneous and symmetric, indicative of no significant structural disorder. **c**, Topography of the same region in Fig.2 b. The right panel shows the dI/dV map for comparison. While there is nematic domain boundary as marked by yellow dashed line (right panel), the atomic lattice (left panel) does not show noticeable changes across the domain. **d**, Temperature dependent topography taken at the same region (upper panel) and their corresponding FFT (lower panel), showing no observable lattice changes. STM Tunneling condition: $V = 100$ mV. $I = 20$ pA.

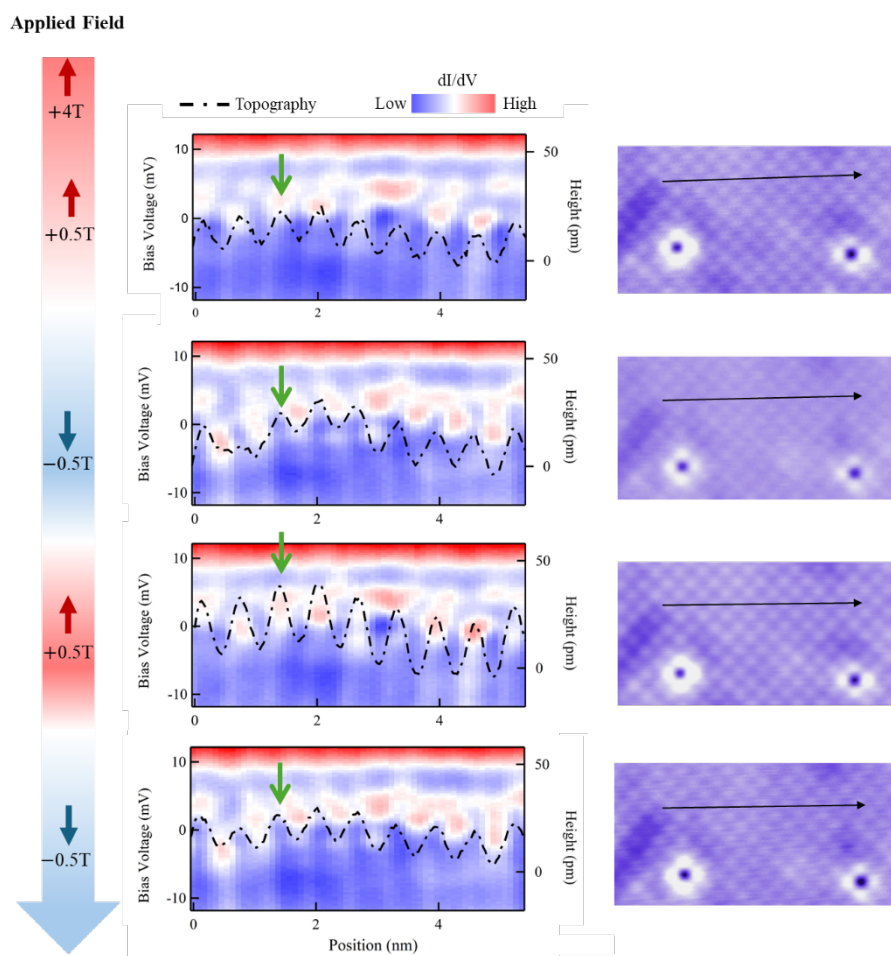


Supplementary Figure 2. Raw and two-fold symmetrized QPI maps. a, Raw QPI maps at selective energy. **b,** Processed QPI maps after standard two-fold symmetrization.

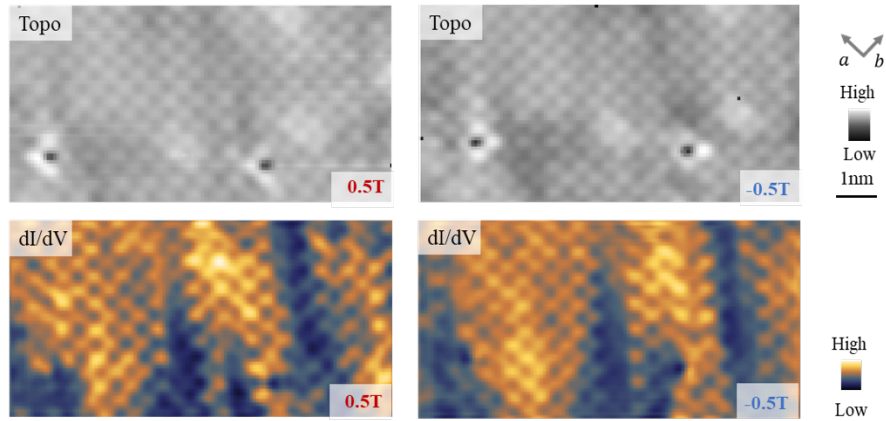


Supplementary Figure 3. Non-observation of contrast reversal with Pt-Ir tip. a, Topography taken at the region of our focus. The position of the linecut is marked. **b,** dI/dV ($V=0$) conductance along the linecut. There is no phase shift between $\pm 0.5T$, in sharp contrast to Fig. 4b. **c,** Intensity plot for dI/dV linecut. At $\pm 0.5T$, the topographic corrugation (black dashed curve) and dI/dV modulation do not show any noticeable change.

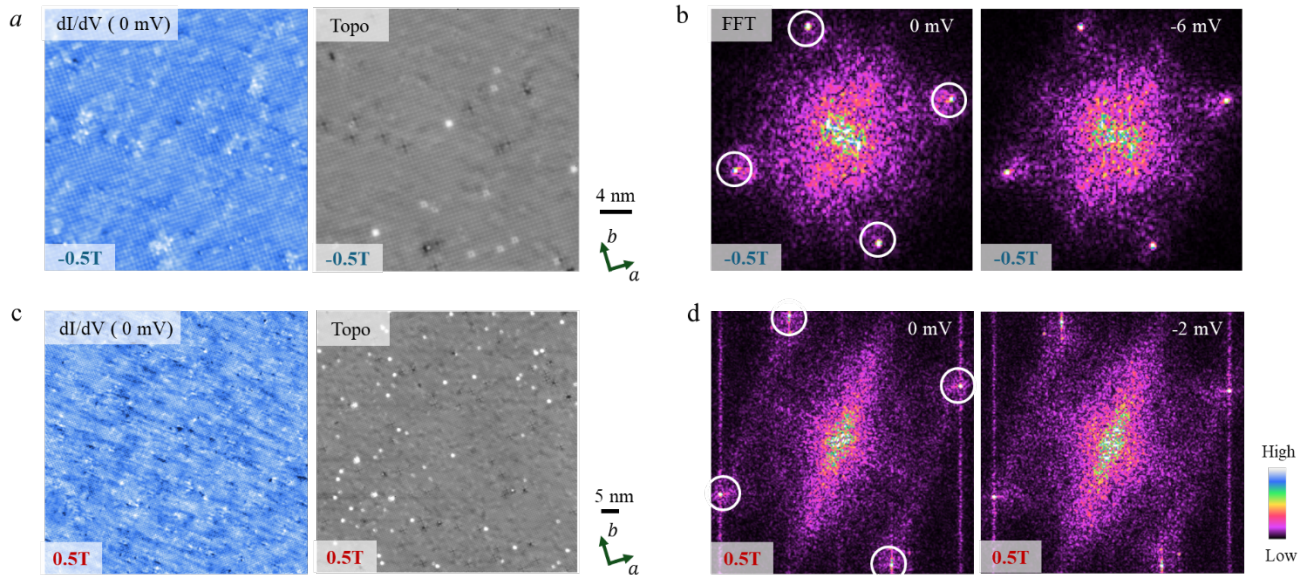
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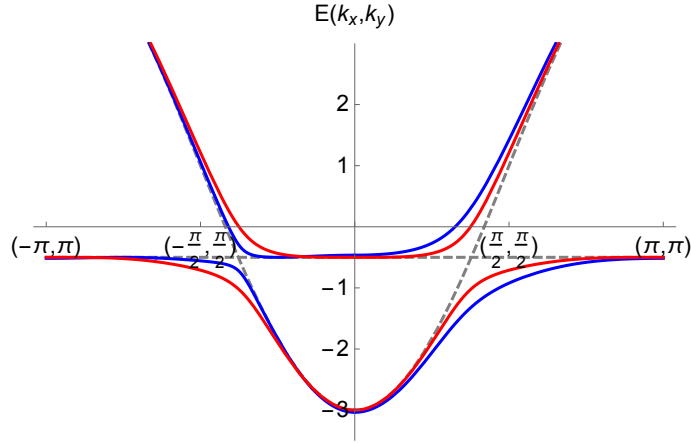
Supplementary Figure 4. Contrast reversal with Ni tip. Data is taken at region II (Fig.4d). The schematic on the left column shows the applied magnetic field in temporal order. Field is perpendicular to ab plane. A 4T field is first applied to polarize the sample and tip. At each field, the dI/dV intensity plot (left panel) and the corresponding topography (right panel) are shown. In the dI/dV intensity plot, the topographic height is drawn with black dashed line. The green arrow points to the same location: At 0.5T, the dI/dV conductance shows signal enhancement (red), while at -0.5T, it shows signal suppression (blue). In the topographic image, the black line labels the position of linecuts. STM tunneling condition for dI/dV linecut: $V = 30$ mV. $I = 170$ pA.



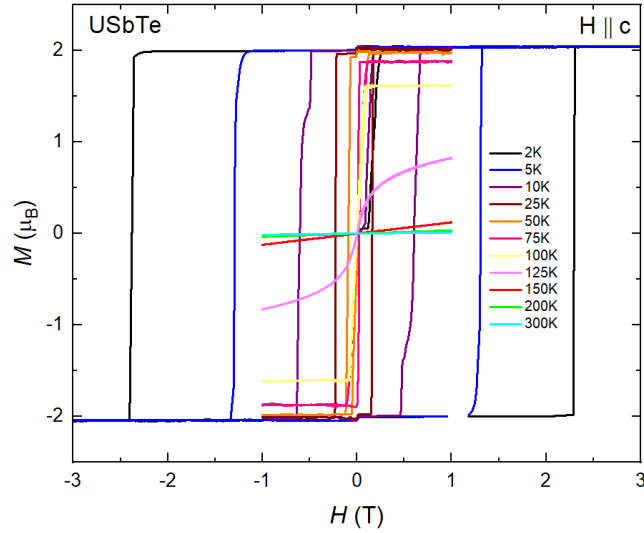
Supplementary Figure 5. Zoomed-in dI/dV ($E = 2\text{meV}$) map with Pt-Ir tip. Data is taken in the same area. The nematic pattern is along the vertical direction and does not change while the magnetic field is flipped. STM tunneling condition: $V = 10\text{mV}$. $I = 180\text{ pA}$.



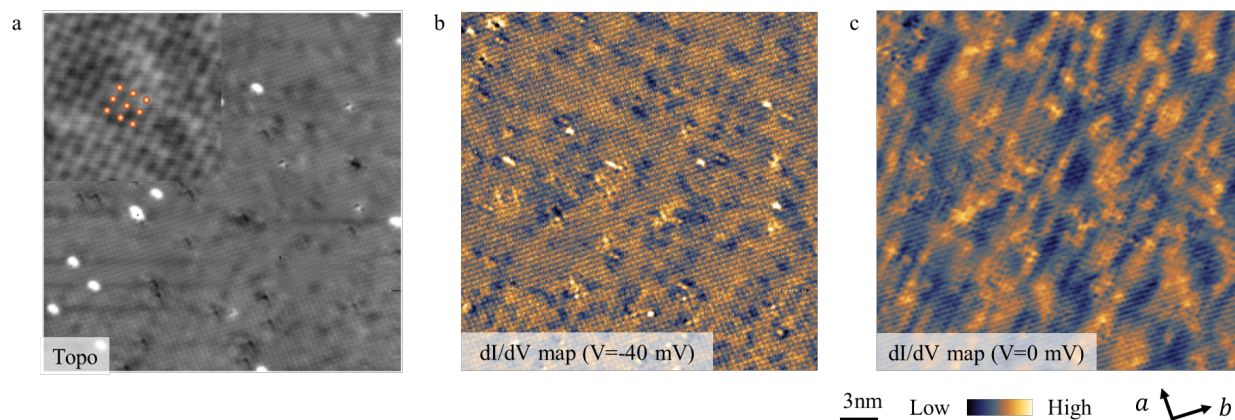
Supplementary Figure 6. Spectroscopic maps with spin-polarized Nickel tip. **a**, Real space dI/dV map at 0meV (left) and topography image (right) under -0.5T . **b**, Fourier-transforms of dI/dV maps at different energy levels under -0.5T . Bragg peaks are marked by white circles. **c**, Real space dI/dV map at 0meV (left) and topography image (right) under 0.5T . **d**, Fourier-transforms of dI/dV maps at different energy levels 0.5T . Bragg peaks are marked by white circles. Spectroscopic maps at 0.5T show prominent $C4$ symmetry breaking patterns, in contrast to maps at -0.5T .



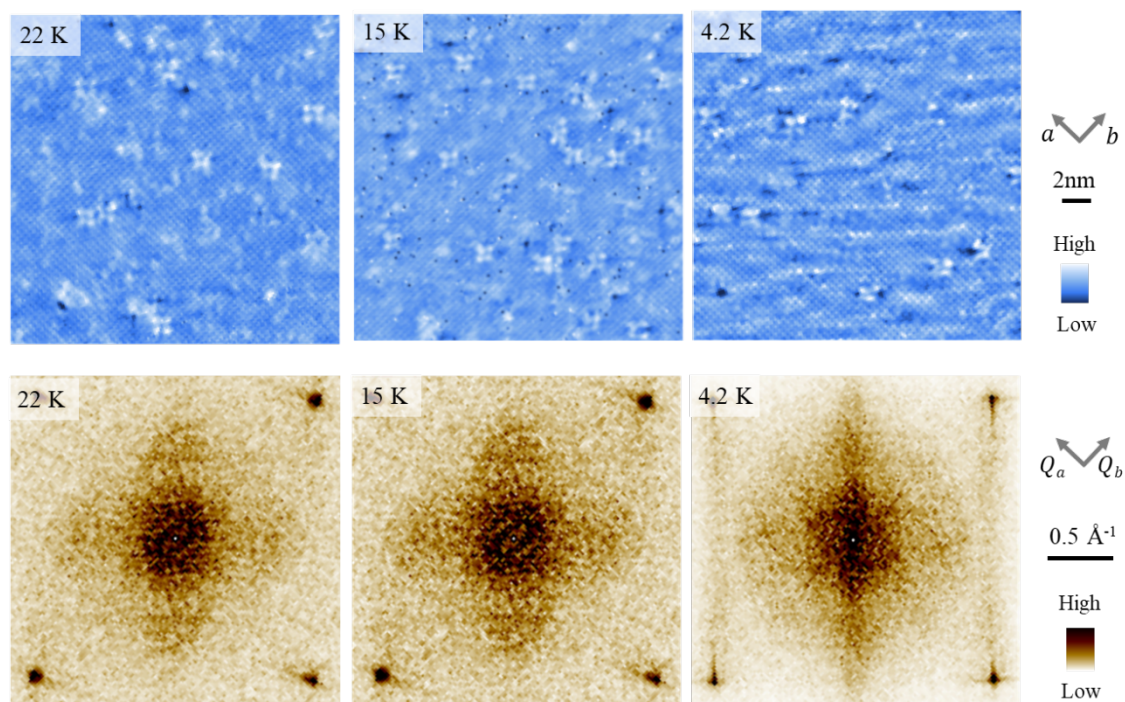
Supplementary Figure 7. Band dispersion of the heavy Fermi liquid phase [Eq. (7)] along the two high-symmetry diagonal directions in the presence of a non-zero nematic hybridization order parameter $\Delta \neq 0$. The red curve corresponds to the case $\tilde{\Delta} = 0$ whereas the blue curve, to $\tilde{\Delta} \neq 0$. Note that only the latter lacks fourfold rotational symmetry. The gray dashed curves are the bare dispersion of the itinerant electrons and the energy of the localized f-electron. To make this figure, we considered a simple dispersion $\varepsilon_{\mathbf{k}} = -2t (\cos k_x + \cos k_y) - \mu$ and $\mu = -1$, $\tilde{E}_f = -0.5$, $\Delta = 0.4$, and $\tilde{\Delta} = 0.3$ (blue curve), with all energies expressed in units of t .



Supplementary Figure 8. M - H curves of USbTe at different temperatures under magnetic field along c -axis of crystal structure.



Supplementary Figure 9. Nematicity on Sb termination. **a**, Topography of Sb termination. The Inset shows a Zoom-in image with Sb atoms labeled. **b-c**, dI/dV conductance maps of the same region at bias voltage $V = -40$ mV and 0 mV. Nematic patterns appear at the Fermi level. Data are taken at 4.2 K.



Supplementary Figure 10. Temperature dependence of dI/dV ($V = 0$ mV) maps and FT-dI/dV maps. Rotational symmetry breaking features appear at 4.2 K and get suppressed above 15 K.

$\langle f^\dagger d \rangle$	$A_{1g} (d_{z^2})$	$B_{1g} (d_{x^2-y^2})$	$B_{2g} (d_{xy})$	$E_g (\{d_{xz}, d_{yz}\})$
$A_{2u} (f_{z^3})$	A_{2u}	B_{2u}	B_{1u}	E_u
$B_{1u} (f_{xyz})$	B_{1u}	A_{1u}	A_{2u}	E_u
$B_{2u} (f_{z(x^2-y^2)})$	B_{2u}	A_{2u}	A_{1u}	E_u
E_u ($\{f_{x(x^2-3y^2)}, f_{y(3x^2-y^2)}\}$) ($\{f_{xz^2}, f_{yz^2}\}$)	E_u	E_u	E_u	$A_{1u} \oplus A_{2u} \oplus B_{1u} \oplus B_{2u}$

Supplementary Table 1. Symmetry classification, in terms of the irreducible representations of the tetragonal group D_{4h} , of the hybridization order parameter $\Delta \sim \langle f^\dagger d \rangle$ arising from the hybridization between U f -orbitals and U d -orbitals.

$\langle f^\dagger p \rangle$	$A_{2u} (p_z)$	$E_u (\{p_x, p_y\})$
$A_{2u} (f_{z^3})$	A_{1g}	E_g
$B_{1u} (f_{xyz})$	B_{2g}	E_g
$B_{2u} (f_{z(x^2-y^2)})$	B_{1g}	E_g
E_u ($\{f_{x(x^2-3y^2)}, f_{y(3x^2-y^2)}\}$) ($\{f_{xz^2}, f_{yz^2}\}$)	E_g	$A_{1g} \oplus [A_{2g}] \oplus B_{1g} \oplus B_{2g}$

Supplementary Table 2. Symmetry classification, in terms of the irreducible representations of the tetragonal group D_{4h} , of the hybridization order parameter $\Delta \sim \langle f^\dagger p \rangle$ arising from the hybridization between U f -orbitals and Sb p -orbitals.