Tomographic mapping of the hidden dimension in quasi-particle interference

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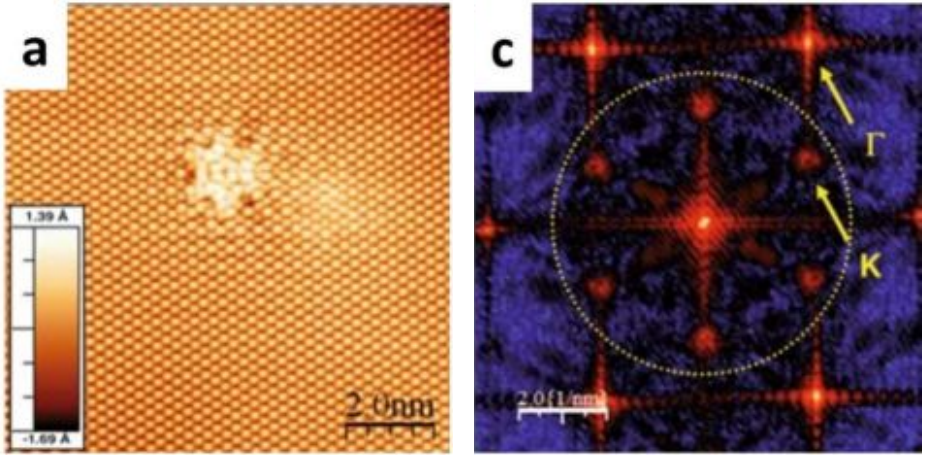
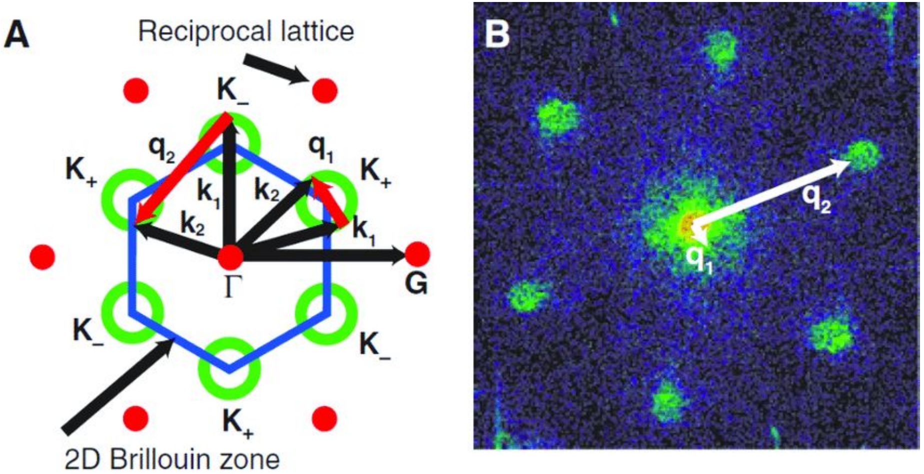
Quasiparticle Interference (QPI)

- A method to extract dispersive information about the electronic states by imaging the standing wave patterns that emerge from scattering off of impurities.

- Fourier transform of STS map directly visualizes the momentum transfer across Fermi surface.

- Inherently limited to quasi-2D systems e.g layered materials, surface states.

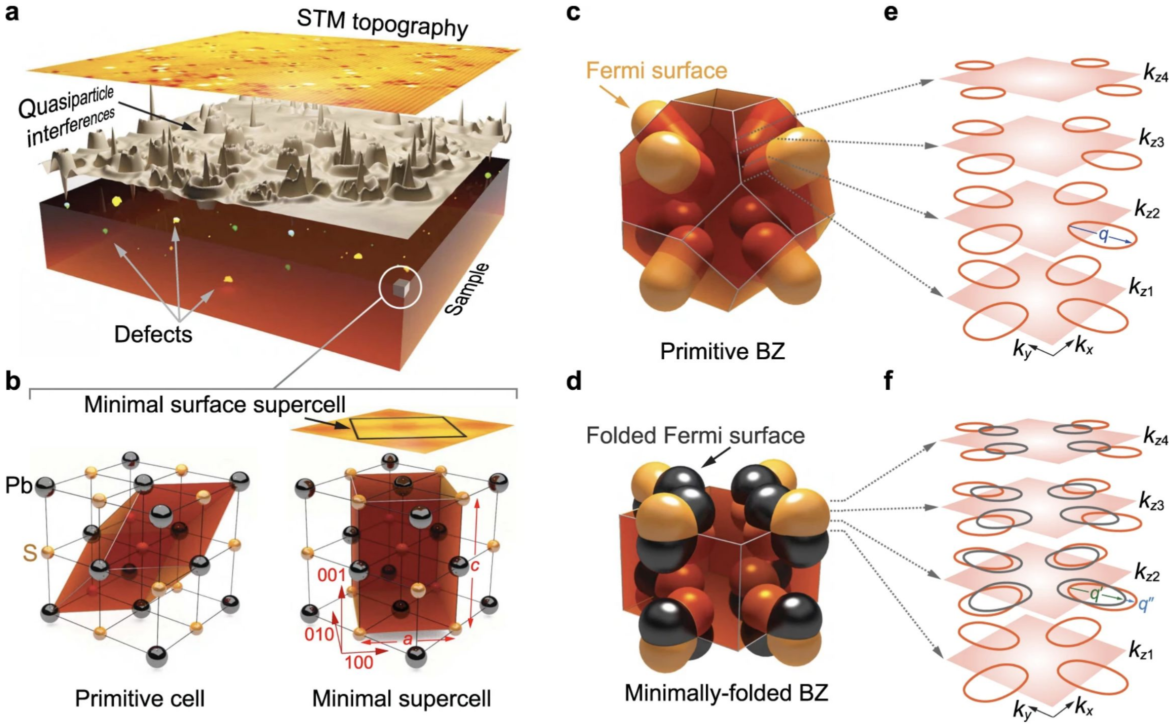




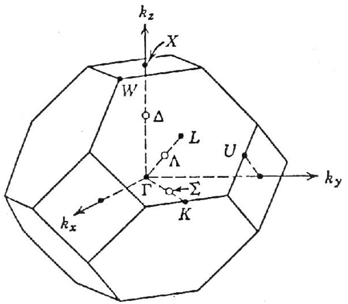
Galena (PbS) Crystal Structure

- Describing how QPI measured at the surface relates to the bulk electronic structure requires addressing what the correct mapping is between surface and bulk reciprocal spaces.

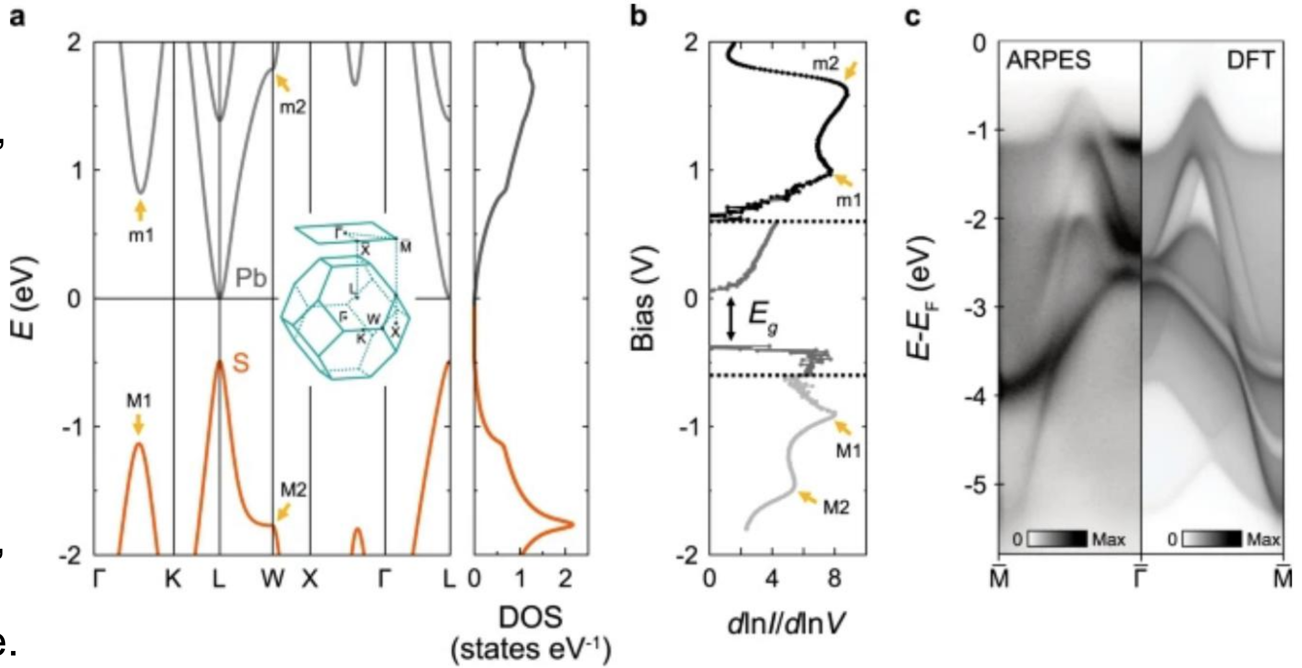
- Minimal supercell that describes surface leads to “folding” of Fermi surface into neighboring BZ, creation of additional Fermi pockets at BZ boundary.



Galena Electronic Structure

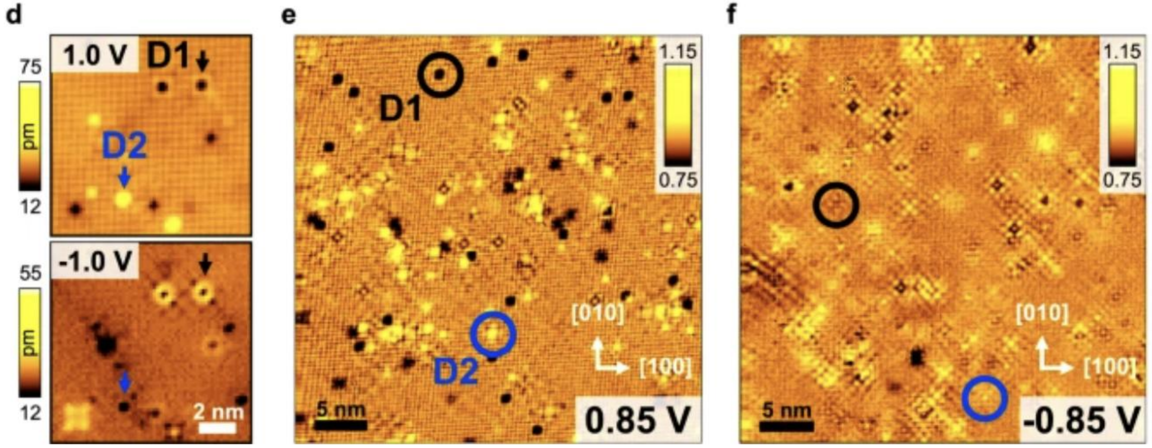


- Calculated band structure shows no states in k_z = 0 plane near VBM or CBm.
- STS shows conduction band pinned to Fermi level, evidence of n-doping.
- Due to rising DOS at positive bias, three set points used in different regions.
- ARPES agrees with theory, shows no surface state, fully 3D electronic structure.



Defects in Galena

- ICP-Mass Spec used to characterize defects, Bi charge donors dominate to make sample n-doped.
- Spatial modulations visible at energies near VBM/CBm, where states have $k_z \neq 0$.



Element	ppm	2σ	Doping
Bi	3322	100	n-type [1]
Ag	1240	157	p-type[1]
Sb	130	61.9	n-type[1]
Cd	44.9	6	p-type[1]
Tl	18.3	5.3	p-type[1]
Se	194.9	20	isoelectronic
Te	34.6	23.6	isoelectronic

Modeling Surface-Projected QPI

1. Use DFT for the supercell to define multi-orbital TB Hamiltonian.

$$H = \sum_{\mathbf{R},\mathbf{R}'} t^{\mu\nu,\sigma\sigma'}_{\mathbf{R},\mathbf{R}'} \, c^{\dagger}_{\mathbf{R}\mu\sigma} c_{\mathbf{R}'\nu\sigma'}$$

2. Extract Bloch eigenvalues and eigenvectors from Hamiltonian in Fourier space.

$$\epsilon_n(\mathbf{k}) \text{ and } |n, \mathbf{k}\rangle$$

3. Compute bare Green's function.

$$G_0(\mathbf{k}, \omega) = \sum_n \frac{|n, \mathbf{k}\rangle\langle n, \mathbf{k}|}{\omega + \mathrm{i}\eta - \epsilon_n(\mathbf{k})}$$

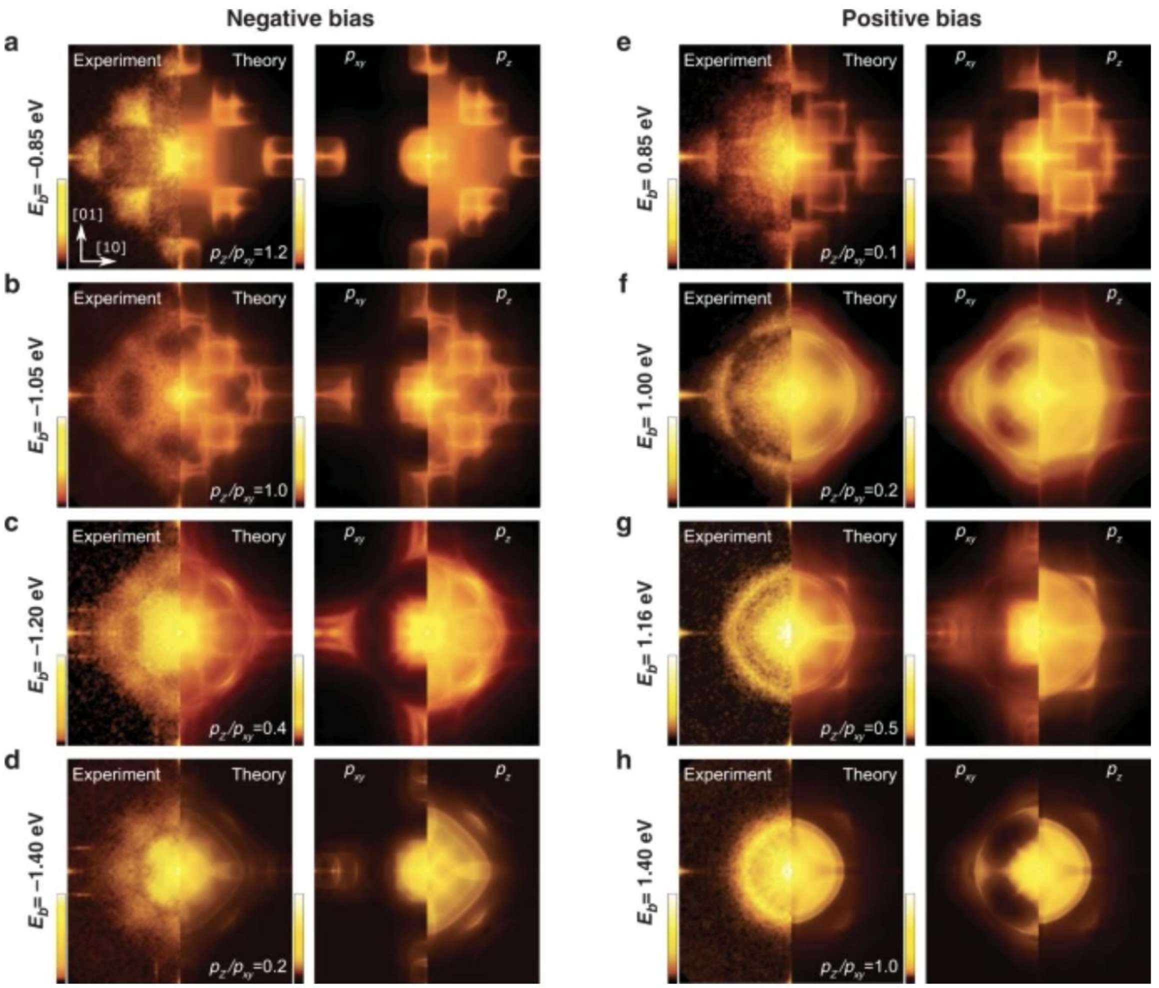
4. Solve for modified Green's function that includes scattering potentials over surface BZ.

$$G(\mathbf{k}, \mathbf{k}', \omega) = G_0(\mathbf{k}, \omega)\delta_{\mathbf{k},\mathbf{k}'} + G_0(\mathbf{k}, \omega) T_{\mathbf{k},\mathbf{k}'}(\omega) G_0(\mathbf{k}', \omega)$$

$$T_{\mathbf{k},\mathbf{k}'}(\omega) = V_{\mathbf{k},\mathbf{k}'} + \sum_{\mathbf{k}''} V_{\mathbf{k},\mathbf{k}''} G_0(\mathbf{k}'', \omega) T_{\mathbf{k}'',\mathbf{k}'}(\omega)$$

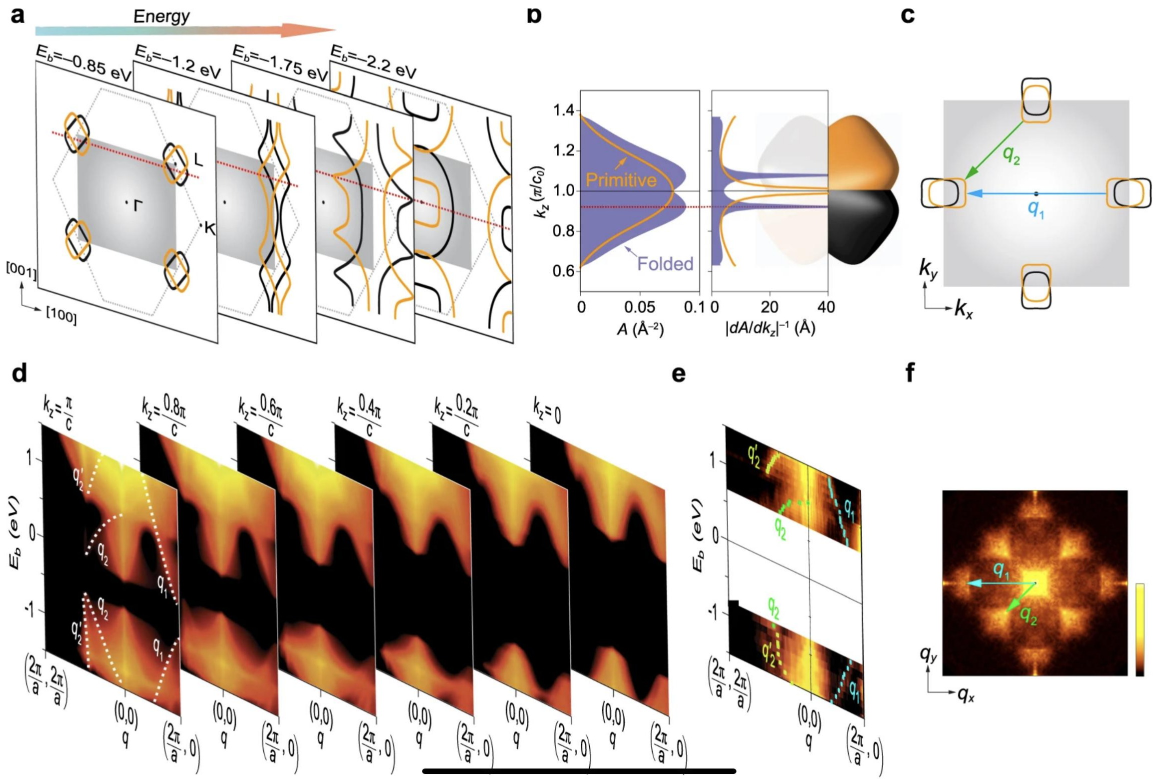
QPI on Galena

- By comparing experimental QPI to theory, can identify patterns that are orbital-dependent.
- Theoretical QPI adjusted by manually tuning ratio of p_z/p_xy scattering to match data.
- At negative, decreasing bias, p_z scattering is weak because impurity states are located at higher energies.
- At positive, increasing bias, p_z strengthens as scattering probability for subsurface impurities increases.



Identifying k_z Scattering Effects

- The QPI signal observed at any given bias voltage is dominated by hotspots in certain k_z planes of the bulk BZ.
- At a given bias, can study curvature of Fermi surface at the boundary to determine dominant k_z plane.
- Demonstrates that observed patterns can only be explained by considering which k_z planes dominate scattering.



Conclusions

- Demonstrated that comparing QPI to theory can reveal aspects of the 3D electronic structure in a material.

- Showed that for systems that can’t be treated as quasi-2D, the k_z plane being considered can seriously affect the resulting scattering patterns.

- Found that bulk electronic structure can be extracted from surface-sensitive measurements.

Extra Slides