Resolving the 2D Structures of New Prospective Quantum Topological Magnets

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This paper represents my own work in accordance with University regulations.

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Abstract

Quantum Topological materials are a class of matter that maintains quantized (discrete) properties under topological (smooth) deformation. More specifically, a material's **band structure** will not have a topological quantum critical point, or intersection between different eigenstates of that material, under incremental change in the system's Hamiltonian. To characterize materials that have such a property, we have resolved the 2D structures of a new QTM candidate, specifically [redacted].

In order to predict topological properties in new materials of interest, probabilistic and spectroscopic properties of the eigenstates ' energies is derived from Gaussian and Lorenz fits, respectively. To investigate materials of interest, we use the UNISOKU Scanning Tunneling Microscope to produce a **tunneling current** between sample and microscope tip. the rate of current provides a Density of States (DoS), which is, through Fourier analysis, then used to extract the material's 2D surface properties.

By analyzing the surface structure as well as verifying topological properties, we have been able to determine which materials (if any) exhibit topological behavior at the quantum-mechanical level. *(results about which magnets do and do not have this property once we have analyzed data).*

Contents

1 Introduction

1.1 QTMs: an Overview

Quantum topological matter refers to a broad class of materials which retain their quantum mechanical properties under such deformation that preserves the material's spatial property. The *quantum* property refers to the discrete set of values a material's characteristic can exist. The *topological* characteristic refers to a property of a space (with a geometric representation) that is constant even when the space itself changes. Topological deformations which preserve such properties are often described as *smooth*, *continuous* or *isomorphic*.

Interest in topological properties of matter at the quantum-mechanical level has so far occupied research resources for only a few decades, and as an urgent area of research confined to the last few years. Such research has led to a fundamentally new understanding of how matter can be manipulated and utilized in developing society.

1.2 Background and Motivation

From all corners of the globe, organizations are taking notice of this very modern branch of condensed matterco. In 2016, the Nobel Prize [1] committee awarded the prize in physics to the discovery of topological properties preserved even under disturbances at the quantum-mechanical level. Meanwhile, the United States Department of Defense [2] has over the last decade offered

[1] Quanta Magazine
[2] DoD Grants and Awards

generous grants to teams researching these materials, their properties and potential applications.

Such research in the private sector will inevitably apply to a public landscape. The topological quantum properties found in both novel and common materials will be utilized to further develop technologies (e.g. more durable quantum computing). A fundamental understanding of how these materials behave at the subatomic level is paramount to exploiting such properties.

1.3 This Investigation

This investigation resolves the 2D structural properties of new quantum topological magnet candidates. The specific magnet investigated in this study is [redacted]. This is of particular interest because of its lattice structure (see Kagome Lattice).

Atomic-level analysis of surface-level topology is used with the UNISOKU scanning tunneling microscope. Data acquisition is performed with Nanonis computer. Analysis is computed through Igor (see ch. 4) and Matlab.

2 Principle Concepts of QTMs

2.1 Quantum Materials

2.1.1 Mechanics

Particles on the sub-atomic level (i.e. electrons) behave fundamentally differently from that of entire objects on the macroscopic level. For electrons, whose precise position and momentum are not simultaneously well-defined, Quantum Mechanics (QM) expresses their behavior as waves (or **eigenstates**). The Schrödinger equations $i\hbar\frac{d\psi}{dt} = [-\frac{\hbar^2}{2m}\nabla^2 + V]\psi$ (time-dependent) and $E\psi = [-\frac{\hbar^2}{2m}\nabla^2 + \mathrm{V}]\psi$ (time-independent) provide the non-relativistic framework on which to describe an electron's state, i.e. the probability of finding a particle in a certain state. The solutions provide a subset of discrete values for the energies that a particle can exist. This range of discrete values is the *band structure* (see 4.1) of a given material, useful for identifying a material's structural properties. Moreover, QM behavior provides the foundation for which *quantum tunneling* and other quantum phenomena occur.

2.1.2 Phenomena

Quantum materials are classified as such because their structures exhibit behavior unexplained by classical physics. The motion of electrons and thus the atomic structure of materials is only explained through quantum mechanics.

One main property of this is that energy levels are quantized so that eigenstates exist at discrete energies. This means that, for a system's set Hamiltonian : (a) the particle/system can *only* exist in a certain range of momentum or coordinate space and *cannot* appear elsewhere, and (b) all eigenstates are non-degenerate. It is the preservation of this last point that characterizes **band topology** (see 2.2).

Entanglement is another QM behavior, which is the long-range interactions between electrons. Electrons couple, or have corresponding movement, even at distances that are macroscopic for electrons. This "spooky action at a distance" coined by Einstein in the 1930s emphasizes the importance of determining a material's general atomic structure and macroscopic behavior (see 2.3).

2.2 Band Topology

2.2.1 Theory

Originally an abstract branch of mathematics, topology is the set of properties of a geometric surface that go unaltered from continuous or smooth deformation. In condensed matter, Band Topology is the theory that uses the quantum-mechanical properties of subatomic matter that give rise to certain properties.

Energy is quantized, meaning that the energy can only be certain discrete amount(s) in each eigenstate depending on the system's Hamiltonian. If this Hamiltonian is altered, the energy levels also change. The topological property of interest at this level, then, is preserving this quantization, which is refered to as *adiabatic continuity*.

2.2.2 Interpretation

Explicitly, **adiabatic continuity** is achieved if the Hamiltonian can be incrementally adjusted so that the topological quantum critical point, or degenerate (equivalent) energy level between the ground and any other state, never occurs. In this case, the band gap , or non-zero difference between energy levels, is preserved, hence quantum topology is preserved.

2.3 Characteristics

Topological quantum materials can exhibit vastly different behaviors, though identifying a material as topological fortifies the network of materials science research and enhances the theoretical framework not yet strongly established. A few notable examples:

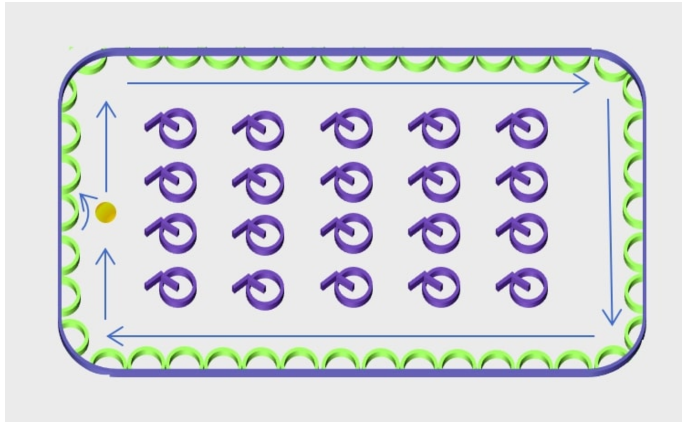

Figure 1: **Topological Insulator**: electron orbits due to the Quantum Hall Effect and topological property give rise to edge conductance.

2.3.1 Topological Insulator

When topological insulators are in a uniform magnetic field, as according to the Quantum Hall effect, all of the electrons are subject to orbit at quantized energies given by $E = \hbar\omega(n + 1/2)$, corresponding to the n^{th} excited state. The inner electrons are in closed orbits, not conducting electricity. Electrons on the edges of the material, however, are in open orbits. This allows electricity to be conducted at the surface edges of the material. This is subject to the Quantum Hall effect, where there is net zero field inside but constant field on surface, leading to topologically preserved orbits for a substantial part of the material.

2.3.2 Superconductivity

Superconductivity is a result of the Meissner effect, which is the expulsion of a magnetic field around such a material. Superconductors are of particular interest in topological materials because they exhibit zero-bias conduction peaks, an important indicator of topological insulators during tunneling analysis[3] (see Tunneling Current, 3.2.2.). This property may also lead to the energy gap that remains a topological property.

2.3.3 Magnetism

Another important quantum property is magnetism, specifically ferromagnetic and anti-ferromagnetic matter. For anti-ferromagnetic behavior, electrons in one lattice iteration have opposite spins. Found in e.g. the Kagome lattice, however, the third electron in this triangular lattice pattern is in a superposition of spin states. This has great implications for quantum computing, where this pattern multiplied many times over gives rise to an exponentially large possibility of states.

3 Scanning Tunneling Microscopy

3.1 Development

Modern classical microscopes employ light as the primary visualization technique. Even with the most precise such microscopes, inspection at the atomic level is not feasible. In 1982, this changed when Binnig and Rohrer utilized the principle of quantum tunneling to construct the first (and 1986 Nobel Prize-winning) Scanning Tunneling Microscope (STM). Over a generation later, STM continues to be widely used to determine a sample's atomic structure.

[3] Chen et. al.

3.2 Principles

3.2.1 Quantum Tunneling

Because electrons behave quantum-mechanically, movement is different on the sub-atomic level. Unlike macroscopic objects, electrons exhibit *quantum tunneling* behavior, which is the capability of wavelike particles to pass through a classical barrier. The exponential solution for the Schrödinger equation mathematically demonstrates a nonzero probability that an electron will appear briefly past the incident point of given classical boundary, defined by the potential V. For each material and microscope, the equations take the form

$$\psi(z) = \psi(0)e^{\frac{-iE_m t}{\hbar}} \tag{1}$$

where m is either s for sample or t for microscope tip. The most general solution in the gap region for the combined system is

$$\psi(z) = \psi(0)e^{-\kappa z} \tag{2}$$

where $\kappa = \frac{\sqrt{2\pi\epsilon}}{\hbar}$. Because this is exponential behavior, the tunneling wave decays to zero exponentially quickly, but still at a distance enough for tunneling to occur. This is the foundational principle on which the Scanning Tunneling Microscope operates.

3.2.2 Tunneling Current

Using tunneling current to reveal atomic structure properties is a method derived from the principle of quantum tunneling. The tunneling current refers to the rate at which elections are moving through the classical barrier. It is driven by applying a *potential bias* or *bias voltage* (Figure 3) to one source of electrons in the system.

In addition to the applied bias voltage , the tunneling current is affected by the width of the tunneling barrier. Distance modulation causes fluctuations in the current. This is useful information for determining both spectroscopic and electronic topological properties properties[4]. For the electrical properties this paper is interested in investigating, maintaining a constant delivers the corollary height information needed to make topological assessments.

Fermi's Golden Rule of time-dependent perturbation theory is

$$R = \frac{2\pi}{\hbar}\left|\frac{M}{2}\right|^2 \rho(\epsilon) \tag{3}$$

where R is the rate of transition.[5] This leads us to the expression for current between systems of tip and sample

$$I = \frac{2\pi e^2}{\hbar}|M|^2 \rho_t(\epsilon)\rho_s(\epsilon)V \tag{4}$$

where $\rho(E)$ refers to the Density of States of the material analyzed (t=tip, s=sample), M is the Bardeen matrix element of perturbation between two interacting states. This is used to calculate the current difference between the continuum of two states[6], namely the charge in the STM tip and that of the sample. M is provided by the integral of the commutator of the sample's wavefunction and the conjugate of the tip's wavefunction.

The net tunneling between the two wavefunctions of tip and sample in both directions:

$$I = \frac{4\pi e}{\hbar}\int_{-\infty}^{\infty} |M|^2 \rho_s(\epsilon + eV)\rho_t(\epsilon)[f_t(\epsilon) - f_s(\epsilon + eV)]d\epsilon \tag{5}$$

[4] Randeira
[5] Griffiths
[6] Chen

where f is the Fermi distribution $\frac{1}{1-e^{\frac{\epsilon}{K_b T}}}$. From here, with the assertions that (a) the Density of States of the tip is in fact flat and (b) the scope of DoS studied is finite, current is derived:

$$I \approx \frac{4\pi e}{\hbar}\rho_t(0)\int_{-eV}^{0}|M|^2\rho_s(\epsilon)d\epsilon^{7} \tag{6}$$

This is the formalism for the Integrated Density of States (IDoS). To extract the shape, or the 2D structure, the Density of States (DoS) is desired, as is derived in our data acquisition (see 3.3.2).

3.3 Experimental Method

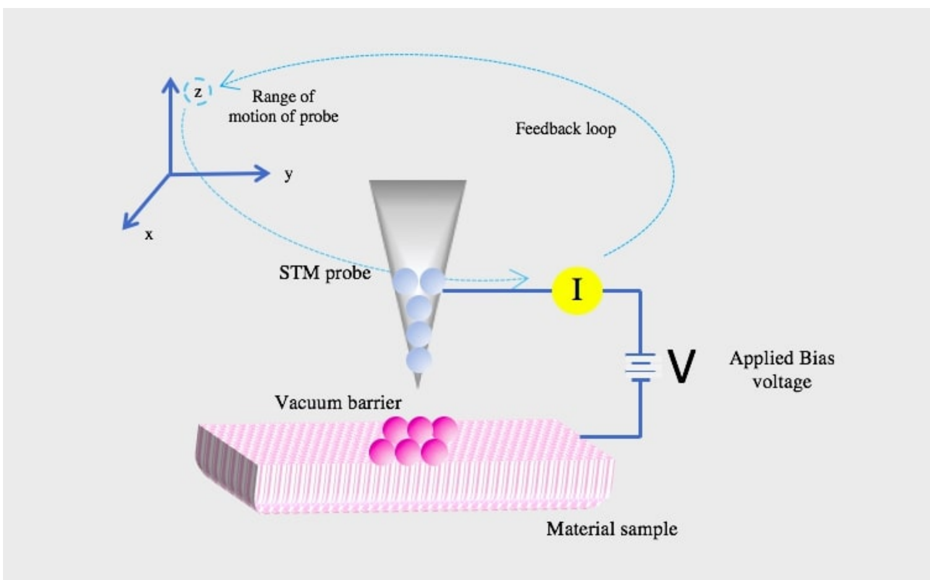

Figure 2: **Scanning Tunneling Microscopy**: Sample schema of STM. A feedback loop keeps the current between sample and tip is kept constant (alters absolute z component, keeps relative z component constant), and scanning occurs in xy directions.

[7] Hoffman 2003

3.3.1 Mechanism

Experimentation using STM relies on the tunneling current. The STM tip is placed at a fixed height of, generally, a few Angstrom away from the sample surface. This distance is appropriate for tunneling to occur. To utilize the tunneling current, In order to be able to perform this integration, one side of the sample has to be *cleaved*, or cut so that the surface's opposite face is flat.

3.3.2 Density of States

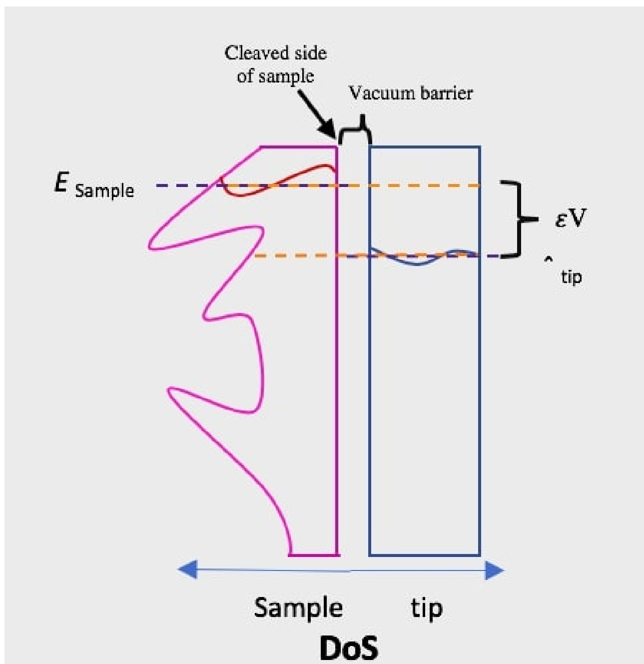

Figure 3: **Tunneling in STM**: When a bias is applied (eV), tunneling occurs so that the filled states of the greater-potential matter tunnel to occupy the other material's empty states. The Density of States (DoS) information from the sample can be gathered from this process, under approximation that DoS of the STM tip is constant.

Tunneling current is produced as a result of a *potential bias* or *bias voltage* applied to the system. This provides information about the *Integrated Density of States (IDoS)*. In order to gather the wavefunction information about the material's structure, however, the local Density of States (DoS) is needed.

This can either be derived, or a small modulation with respect to V can be applied. This results in being able to measure DoS, by

$$\frac{dI}{dV} \propto \rho_s(\epsilon + eV)^{8} \tag{7}$$

where the matrix element M and DoS $\rho_t(\epsilon)$ are, still, approximated to be constants.

$\frac{dI}{dV}$ (conductance) as a function of applied bias eV offers insight into the material's band structure (see 4.1).

3.4 Operation

3.4.1 Sample prep

In order to extract a flat surface for tunneling analysis, the sample has to be properly prepared for cleaving. A 2:1 mix of Torr Seal Resin and Hardener is applied to the middle of a sample no larger than $1mm^2$, to which a plastic cleaving stick no larger in diameter than the sample is attached. The sample is placed in the middle of a copper plate, followed by about an hour of heating on a hot plate. Once heating is done, the part of the sample with Torr Seal is then applied with graphene spray to maintain proper tunneling conductance. After brief drying, the sample is then ready to be loaded, cleaved and scanned.

3.4.2 STM

The Scanning Tunneling Microscope, though fragile, is a powerful tool used to regulate the ideal conditions necessary for a successful scan. When a sample is ready to be analyzed, it first needs to be manually loaded into a vacuum-controlled doc. This ensures that impurities are minimized. The sample is then transported again to the cleaving chamber, cooled by liquid nitrogen.

[8] C. J. Chen

It is cleaved by manually clipping off the stick previously adhered by Torr Seal to the sample. After cleaving, the sample is then loaded into a liquid helium-cooled chamber, kept ideally 4-5K at the coolest depths and 10K at the sample level. From here, the sample can be unloaded, rotated, and any other manipulations between scans.

4 Experimentation

During trials, an array of variables may delay result acquisition. In a majority of cases, even in the most secure vacuum environment, impurities are still found on the sample. During analysis, the impurities cover the surface, eliminating otherwise viable surface area space. In other trials, sometimes a sample is only partially cleaved, rendering the sample itself no longer viable to analyze.

When a sample is used, if sample does not exhibit clear atomic structure (faulty resolution), then the sample goes through up to three rounds of x-y rotation until either a surface with clear atomic structure has been identified.

Before a surface is sent to the liquid hydrogen-regulated chamber to be scanned, a couple of visual indicators are noted. If the STM plastic stick is not fully removed and damaged beyond the capability of removal, then the sample is not used at all. If a sample appears dull/is not notably metallic, possible defects/impurities are expected. If the sample, however, appears metallic after cleaving, this is correlated with a higher success rate in finding clean surfaces.

4.1 Technologies

Careful analysis of materials requires the use of many technologies. The two I have mainly used over the SRC program are Matlab and Igor. Igor and Matlab are both data-analysis and visualization software programs. Igor is compatible with STM software and can keep track of STM and sample specifications. Matlab is a wider-used program capable of producing easily-customized figures. Both are capable of producing Lorenz (spectral) and Gaussian (statistical) plots of surface-structure behavior.

Another example of software briefly managed over the summer is WSxM, a Windows-based STM data processing software. It can perform such manipulations as Fourier Transform, which is used to derived the momentum-space and therefore structural properties of a material at the atomic level. For Mac/Linux users, enabling TeamViewer with Windows is a useful method.

Software programs Vesta and VASP are used for theoretical imaging and manipulation. Vesta is a free-access program suitable for atomic structure imaging of registered compounds (available widely through Springer materials). VASP is a program available by license, constituting the imaging with added programming capacity.

The STM used in lab is the UNISOKU, used in tandem with computer software Nanonis. UNISOKU consists of all of the aforementioned parts of the STM, and all raw data acquisition as well as UNISOKU operation is dictated to the STM equipment through Nanonis.

5 Data Analysis

5.1 Band Structure

The **band structure** is the spectrum of allowed energies for the different excited/ground states in a given system upon applying different biases. A **band gap** is the difference in energy between eigenstates . When a band gap is nonzero and finite, the states are non-degenerate. If this property is preserved, the band topology is also preserved.

A method for visually resolving the band structure is to construct a material's **Brillouin Zone** (**BZ**), which is the reciprocal lattice constructed by performing a Fourier transform on real space. In the BZ, we are able to calculate and plot the energy in momentum-space k. k vs E band-structure visualization is of particular interest because the allowed energies of different states are visually represented.

Graphically, points of **high symmetry** in the BZ are important because they indicate critical areas of behavior. **High-symmetry points** (e.g. trivial Γ) are invariable points under a high order of rotation. In the Brillouin Zone , such points map onto themselves in reciprocal space, indicating features that are consistent in multiple rotations when a structure is decomposed into all of its individual patterns. Such behavioral symmetries are notable when in the context of **momentum space** (see 5.2).

5.2 Landau Levels

When a material is in a magnetic field, the kinetics of its electrons due to the quantum hall effect are affected. When the Landau gauge is factored in, which preserves time-reversal symmetry, the energy of the electrons can be reduced to a one-dimensional oscillation, where the energy levels are $E_n = \hbar\omega(n + \frac{1}{2})$. This produces the Landau levels.

Landau levels are visualized through E-vs-conductance plots, where the peaks correspond to the Landau levels.

In topological materials, Dirac-Cone representaion of LLs indicate said quantized energies as well as where a band gap would be. In **momentum-space** , derived from the Fourier Transform of position-space on a wavefunction, the relationship between eigenenergies and movement can be analyzed.

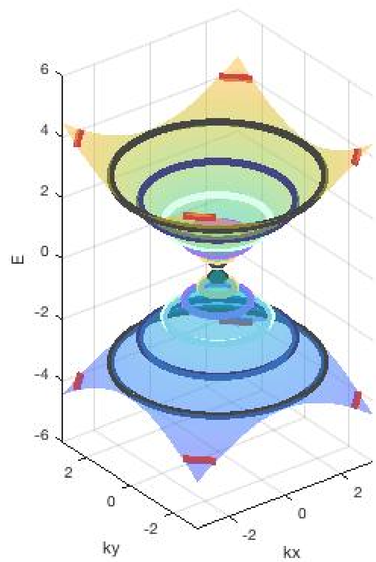

Figure 4: **Dirac-Cone LLs**: Example of two-dimensional momentum in relation to LLs (in varying colors). At the plot origin–where the cones almost appear to meet–would be the point of the band gap.

5.3 Kagome Lattice

Researchers in this particular lab investigate materials that have a characteristic Kagome lattice, which consists of one layer of triangulated atomic arrangement. This lattice has exhibited topological properties in experiment, and its theoretical application to quantum computing makes it an exciting class of materials. Because of the triangulation of the atoms, an anti-ferromagnetic Kagome lattice will have two opposite-spinning electrons with one electron in superposition. This superposition leads to the theoretical application.

[redacted]

Figure 5: **Kagome Lattice Structure in** : The Mn atoms in a layer of the material create the lattice, introducing exciting potential applications for it from this physical property.

6 Results

For magnet [redacted], Landau levels can be detected. This constitutes [redacted] as a promising possible topological magnet. The magnet also exhibits near-consistent LLs within the range of 100-150V for entire tested range (0-10T) of magnetic field. This is a prime indicator that this magnet retains its topological properties within this range of potential bias.

The Kagome lattice is also identified through STM. As theoretically modeled, the microscope detects the topography at the atomic level of the material, which has a visual representation of the lattice structure. This is an indicator of the class of materials it belongs to as well as behavioral properties that make it an exciting material to investigate in up-and-coming technologies.

7 Discussion

The landau levels detected in [redacted] are defined well, suggesting it may be a good topological magnet candidate. This research inches us closer to

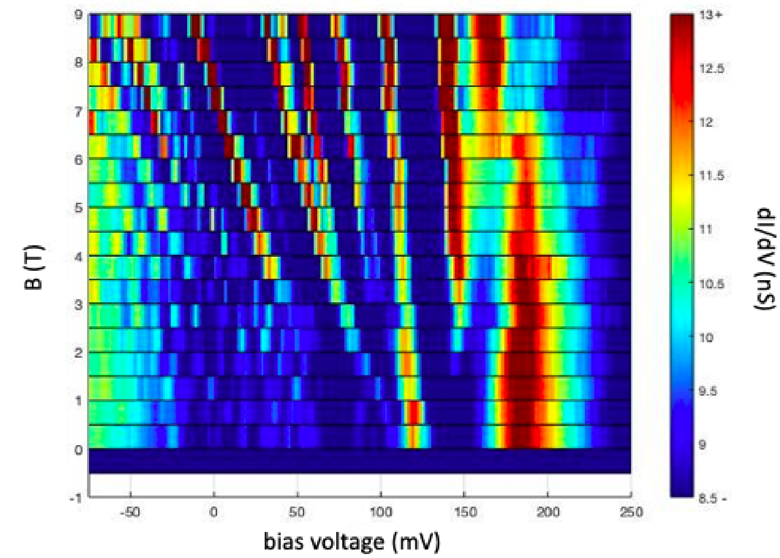

Figure 6: **Landau Levels (LLs) of** : LLs are graphically visible at any local maxima of $\frac{dI}{dt}$ (colorbar) with respect to the potential bias (V). LL peaks are found through entire range of tested magnetic field (T).

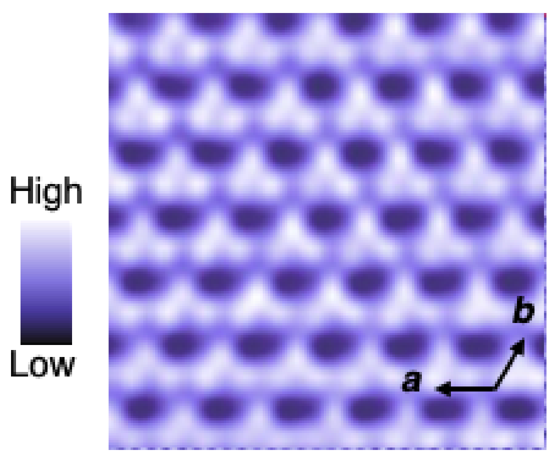

Figure 7: **Lattice Sructure of** : An STM scan of a section of the material demonstrates the Kagome lattice structure linked to promising topological and quantum properties.

defining the theoretical basis for quantum topology and how it may be beneficial in developing society. Further research will focus on determining the magnet's classification as well as establishing a theoretical basis for topological behavior.

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This work is ongoing for the 2019-2020 academic year in the Hasan lab.

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