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Numerical predictions for a topological insulator: an SSH chain on InAs(111)A

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Abstract

Topological insulators are materials that are insulating in the bulk, but exhibit conductive states at the boundaries. An example of a topological insulator is the SSH chain. In this thesis, we use a muffin tin model to systematically investigate the hopping parameters, for which an non-trivial, trivial, and delocalized phase is manifested by In adatoms on an InAs(111)A platform. We find that this behaviour is manifested by an SSH chain of 8 artificial atoms, with each artificial atom consisting of 6 In atoms, for the hopping parameters $t_1 = 5a'$ and $t_2 = 2a'$. We anticipate that this thesis provides a stepping stone for the future experimental realization of an In adatom SSH chain.

Contents

1 Introduction

In physics, observation and experimentation are the primary methods for investigating new and yet unexplained phenomena. From the observation of the orbits of planets to the experiments confirming the existence of time dilation, most theories can be tested by setting up hypotheses and then performing the right measurements in order to better understand physical phenomena and properties of materials. This was all fairly easy because most experiments were done on scales that are easily manipulated and or measured. This had the consequence that the laws of nature could be studied by (artificially) creating the right circumstances for the phenomena to be studied in a controlled environment.

This ability to create a controlled experiment was put to the test by newer and more extreme theories and phenomena. From the study of vacuum environments to the study of materials at extreme temperatures, physics became incrementally more difficult to observe and measure. One particularly difficult to study topic is quantum physics. This difficulty is due to the incredibly small scale on which the phenomena need to be studied to manifest themselves. Luckily large steps have been made in the area of technology which enabled us to study those extremely small length scales[1][2][3]. This has enabled us to create and measure on an atomic scale, in order to perform quantum experiments[4].

The invention that we will use in our experiment is the Scanning Tunneling Microscope or STM for short. This device uses a very sharp needle and the phenomenon of quantum tunneling to measure objects at a subnanometer resolution. This enables us to depict atoms, and using Scanning Tunneling Spectroscopy we can measure the energy spectrum of the atoms and their surrounding. This energy spectrum gives us the Local Density Of States, or LDOS[5]. This LDOS gives us the amount of states present at a location, and coincides with the probability of finding an electron at that location. The STM can also be used to manipulate singular atoms, which makes it possible for us to perform experiments on a system of atoms that is tailor-made for that particular experiment, a so-called artificial lattice.

One experiment one might do using an STM is the creation of a topological insulator. A topological insulator is a material that depending on the chosen parameters is insulating, conducting, or a mix of both. In this mix, the bulk of the material is insulating while the fermi level states are present at the boundaries. One topological insulator that lends itself well for study using an STM is the SSH chain[6]. The SSH chain is a chain of atoms with different interaction strengths. Depending on the chosen interaction strengths between the atoms, the chain manifests a delocalized, trivial or

nontrivial phase. The interaction strengths are dependent on the distances between the atoms and can thus be manipulated using an STM. This makes the SSH chain an ideal system to study.

This thesis investigates the feasibility of creating an SSH chain made of artificial atoms using an STM. The artificial atoms are comprised of 6 In atoms and are placed on an InAs(111)A lattice. This lattice has been chosen due to its energy resolution, which is higher than the energy resolution of the previously used system of CO molecules on a Cu(111) substrate. We will calibrate the muffin tin model for this system using experimental data from Fölsch et al.[7], after which we will show the energy spectra of the chain for different parameters.

2 Theory

2.1 Scanning Tunneling Microscopy

The Scanning Tunneling Microscope (STM) was invented by Gerd Binnig and Heinrich Rohrer while working at IBM Zürich[1]. This invention made it possible to create an image on which individual atoms are visible, this makes the study of materials on a nanoscale possible.

The workings of an STM are simple. The STM consists of an atomically sharp needle, which is the size of one atom at the tip, a motor, a sample, and an electronic measuring and control circuit. The STM starts its measurement by letting the needle approach the sample's surface. The needle is in feedback when a current starts to flow from the needle to the sample. This current is in the order of nA and depends exponentially on the distance between the tip and the sample. The current can be kept constant by adjusting the tip height using a feedback loop. If we move the STM tip in the x or y direction we might encounter an atom. This means that the tip-sample distance decreases, and as a consequence that the tunneling current will increase. At this moment a feedback system engages a piezo motor which will adjust the height of the STM tip above the sample such that the current remains constant. This change in height is measured along with the lateral position of the needle. After completing a full survey of the field of view, we are left with all the data we need to compile a full topographical map of the sample on an atomic scale. For a more detailed overview of scanning tunneling microscopy, we recommend the book from Bert Voigtländer**??**, and the book by Julian Chen[9].

2.2 Moving atoms

The fact that we can now distinguish atoms on a lattice by observing the topography of the lattice has also made it possible to start thinking about manipulating singular atoms on that lattice. This was famously done by IBM in order to make the film 'a boy and his atom' in 2013[10]. Here the researchers used an STM to make a one minute long stop motion film by manipulating CO molecules on a copper substrate. But the manipulation of atoms has also allowed the building of nanostructures to study electron configurations, the study of more complex quantum systems such as hexagonal lattices[11] and fractal geometries[12].

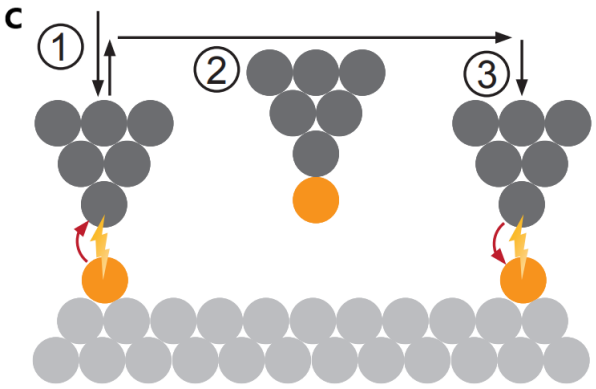

Figure 1: The vertical manipulation of an atom by forming a reversible chemical bond. Step 1 is the approach of the tip and applying a large voltage to the tip causing the adatom to attach itself to the tip. Step 2 shows the moving of the atom to the desired position. Step 3 shows the deposition of the atom onto the substrate.

The moving of atoms is done by bringing the STM tip close to an atom by applying a higher current to the tip. This current can lead to a pulling effect by inducing an attractive interaction between the tip and the atom, a pushing effect can be created by the use of a repulsive interaction between the atom and tip[13][14]. Using these interactions we have three methods for moving an atom. The first method is hovering the tip above the target atom and applying a voltage such that a pulling force is applied to the atom. After the application of the high voltage, we tow the atom to its desired position[15][16]. The second method is applying a voltage to the tip such that the target atom is repulsed by the tip and is pushed by the tip toward its desired position[17]. The third method is temporarily bonding the tip to an adatom so the adatom is pulled off the substrate and hangs onto the tip,

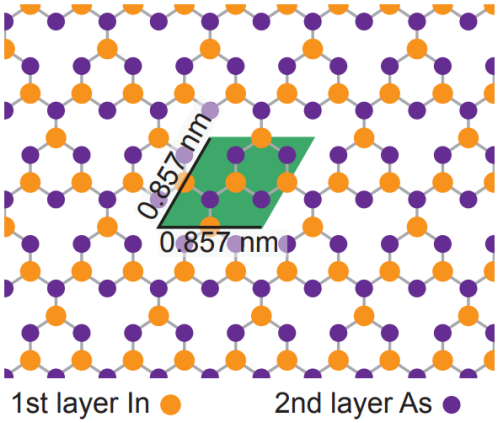

Figure 2: A graphical depiction of an InAs substrate with the unit cell in green. The top layer is made up of In atoms (orange), the second layer consists of As atoms which are colored purple.

this is depicted in figure 1[18]. Now the tip is moved to the desired position and an opposite voltage is applied so that the atom detaches from the tip and lands on top of the substrate in it's desired spot.

2.3 The substrate

In our experiment we will use an InAs(111)A-(2x2) substrate, But what does this mean? The InAs gives us the information of what atoms our substrate is constructed. The A on the end provides the information that the top layer of the substrate is of the A-type, this means that this layer is made up of In atoms. The last piece of information is hidden in the (2x2) indication. This means that we have a (2x2) In vacancy reconstruction, of which the unit cell is indicated in figure 2. The InAs lattice constant is $a_0 = 0.606$nm with a vacancy spacing of $a' = \sqrt{2}a_0 = 0.857$ nm.

2.4 The SSH chain and topological insulators

The final question to be answered in order to understand this thesis is: what is an SSH chain and why it is important? The SSH chain was first discovered by Su, Schrieffer, and Heeger who published their findings in 1979[6]. They were theoretically investigating the simplest linear conjugated polymer, Polyacetylene. They discovered that this molecule displayed very interesting electronic structures and bonds. Later it was discovered that these properties meant that the SSH chain is a topological insulator[19].

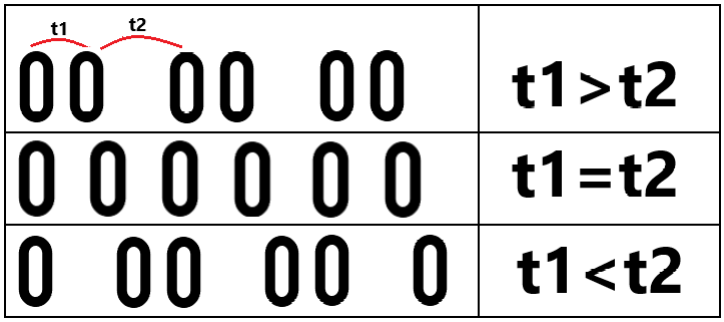

Figure 3: A graphical depiction of the trivial chain $t_1 > t_2$, the delocalized chain $t_1 = t_2$, and the non-trivial chain $t_1 < t_2$.

Topological insulators were first theorized in 1987 by Oleg Pankratov who predicted that symmetry protected edge states can occur in certain materials[20]. This means that the material or configuration behaves as an insulator on the inside but has conductive states on its surface or edge. For a SSH chain, this means that there are fermi level states present at the chain's boundaries while maintaining an insulating bulk. This we call a topological boundary state. For a 2D topological insulator, for example, a square, this means that the vertices are conducting and the surface is insulating, and in a cube, the surface is conducting while the interior is insulating. Whether this behaviour is manifested by an SSH chain depends on the bonds between the atoms, commonly referred to as the hopping parameters t_1 and t_2, when using the tight-binding approximation. We will continue to use this naming convention due to its usefulness. Calculations have predicted that we find the trivial variant when $|t_1| > |t_2|$, as depicted in figure 3. When the hopping terms are equal, so $t_1 = t_2$, we have the delocalized variant of the chain. The nontrivial variant, which can manifest topological boundary states is present for $|t_1| < |t_2|$[21]. Due to the possibility of placing atoms at any vacancy on the substrate, we are able to vary the distance between our artificial atoms. When we place the artificial atoms close to each other we find a large hopping parameter. If we place the artificial atoms further from each other we reduce the hopping parameter. This means that we can vary the hopping parameters by manipulating the distances between the artificial atoms.

The experimental investigation of the SSH chain has progressed since 1979, in 2018 Gröning et al. found that the SSH model can be realised in edge-extended graphene nanoribbons[22]. In the same year, Rizzo et al. realised a graphene nanoribbon lattice on an Au(111) substrate, which manifests non-trivial one-dimensional topological phases[23]. In 2020 Huda et al.

built an artificial SSH chain on an atomic level by using an STM in order to construct the chain and vary the hopping parameters. This experiment was realized using chlorine vacancies on a Cu(100) lattice[24]. STM experimentation on the SSH chain has also been done by Cheon et al. who used a Si(111) platform on which Indium atoms were deposited[25]. This experiment shows that the SSH chain can also be manifested by metallic wires made out of Indium. In this thesis, we will assess the feasibility of using In adatoms on InAs(111)A to further the investigation of topological phases manifested by an artificial SSH chain.

3 The model

For the numerical simulation, we will be using a muffin tin model written in Python. This model was originally developed by Rian Ligthart, Ingmar Swart and Stephan Zevenhuizen in 2019 in order to perform calculations on a system of CO molecules on a Cu(111) substrate. The Python scripts can be obtained upon reasonable request by contacting the authors. We start our calculations by defining our lattice. This is done using a script which allows us to select a vacancy on our substrate where an In atom will be placed. After we finish the placing of the atoms, the script creates s simple coordinate file which contains the positions of the placed In adatoms. Our next step is performing the muffin tin calculations. For this, we load our coordinate file into the eigenvalue script. This script will then assign a Gaussian potential to each atom. The Gaussian potential can be adjusted for different substrates and adatoms using the Gaussian height to modify the depth or height of the potential. The width of the Gaussian potential can be adjusted by changed by altering the full-width at half max of the potential. Together, all the placed potentials form a potential field for which the Schrodinger equation is then solved numerically in order to find the eigenvalues. We will perform these calculations for 400 wavefunctions to keep the duration of the calculations relatively short, while still showing enough details.

After the calculation of the eigenvalues, we can create a Local Density of States (LDOS) map on which we can pick a position to take a closer look at the local energy spectrum. The LDOS represents the local density of states which is the number of states that are present at a specific location. If the LDOS is high, then there are many states present, which means that there is a high probability of finding electrons at that specific position. A low LDOS means that there are few states present at a location, which tells us that we have a low probability of finding electrons at that location.

Because the muffin tin model was originally written for a system of CO

molecules on a Cu(111) substrate, the Gaussian potentials were originally repulsive. By adjusting the Gaussian potentials to be negative we can modify the model to simulate an attractive potential, which we need to model In adatoms on an InAs(111)A substrate.

4 Results

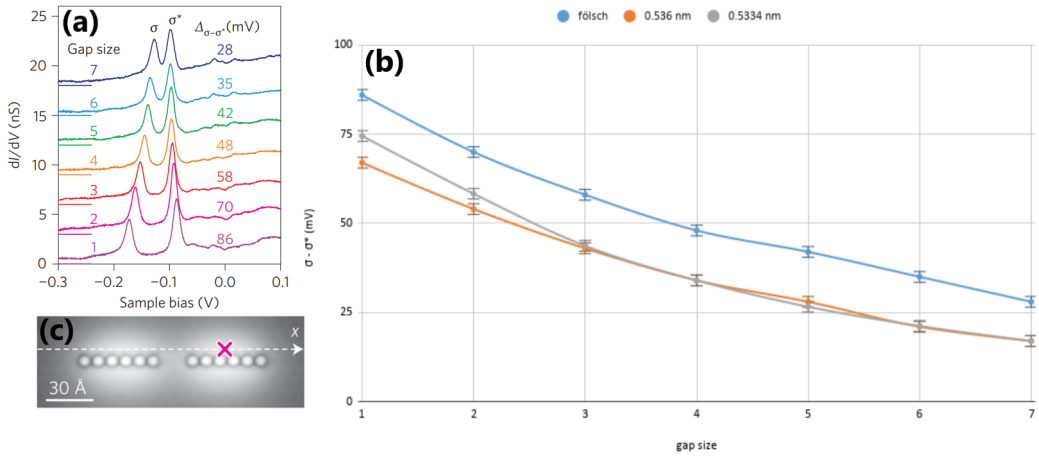

Figure 4: (a)Di erential conductance spectra measured on arti cial atoms with varying gap size from Fölsch et al.[7]. (b)The splitting as a function of gap size for di erent FWHM with a gaussian height of -2.0eV. (c) Topographic STM image of two arti cial atoms separated by a gap of two vacancy sites from Fölsch et al.[7].

4.1 Model calibration

Before we can investigate how to construct an In SSH chain we must determine what the model's parameters have to be. The model parameters are the full width at half max (FWHM) of the muffin tin potentials, the accompanying Gaussian height, the energy shift, and the scaling parameter. In order to determine the optimal values for the parameters, we will use experimental results by Fölsch et al.[7]. In their experiment, Fölsch et al. placed two In artificial atoms, consisting of 6 In adatoms each, on an InAs(111)A substrate. These artificial atoms are placed head-on as seen in figure 4c. The energy spectrum of these artificial atoms shows two peaks, as depicted in figure 4a. The smaller peak is the bonding peak (σ), while the larger peak is the anti-bonding peak($\sigma*$). From the energies at which these peaks are located, we can calculate the peak splitting ($\Delta_{\sigma-\sigma*}$), which is the energy

difference between the peaks. Looking at figure 4a we notice that when we bring the artificial atoms closer to each other (the gap size becomes smaller), the peak splitting becomes larger. We can graph the relation between peak splitting and gap size, this is done in figure 4b. For the calibration of the FWHM and the Gaussian height, we will simulate the artificial atoms in the same configuration as used by Fölsch et al. and measure the peak splitting for a range of parameters. We will then look at which parameters lead to the results which are closest to the results from Fölsch et al.

Looking at our simulated results plotted alongside the line from Fölsch et al., as depicted in figure 4b, we see that the lines for a FWHM of 0.536nm and 0.5334nm all have a similar slope. We also observe that the simulated data have a vertical offset when compared to the experimental data. The differences between the numerical values and the values from Fölsch are on average 14.7nm for the orange line and 13.1nm for the blue line, a graph with the splitting for more values of the gaussian height can be found in the appendix. We conclude that the parameters Gaussian height -2.0 and a FWHM of $0.6224a'$ (= 0.5334nm) are the best fitting parameters for our model.

Now with the correct parameters, the investigation of the SSH chain can begin. We will do this by looking at a 2D map of the local density of states (LDOS), and by looking at spectra taken at the middle and the end of the SSH chain.

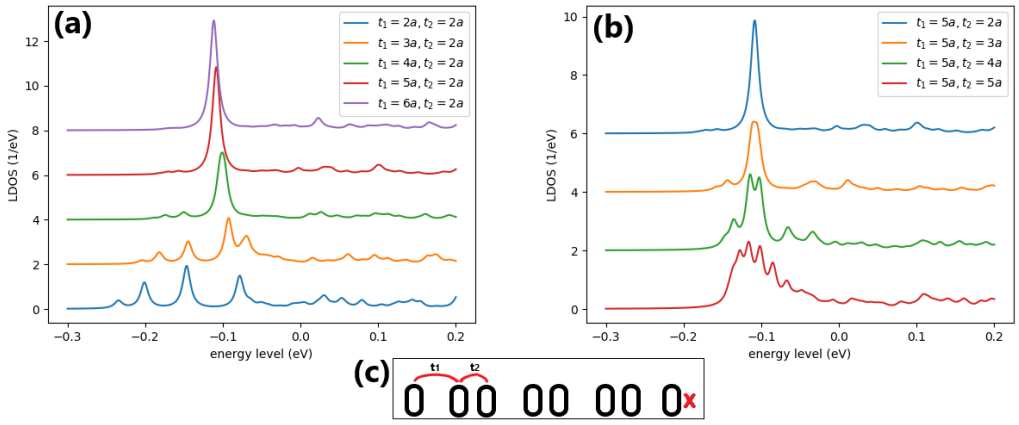

Figure 5: (a)The LDOS spectra for the parameters $t_1 = 2a'$ and $t_2 = 2a'$ to $t_1 = 5a'$ and $t_2 = 2a'$. (b)The LDOS spectra for t_2 varied from $2a'$ to $5a'$ with $t_1 = 5a'$. (c)A schematic depiction of the arti cial atoms with a red cross denoting the position where the spectra are taken.

4.2 The SSH chain for different parameters

Now the model is calibrated for In atoms on InAs(111) we will start our search for the right parameters by looking at an SSH chain made of eight artificial atoms, each consisting of 6 In atoms. These artificial atoms are placed parallel to each other.

In figure 5a we see the spectra taken on the right of the last artificial atom of the chain for different configurations. We start by setting t_2 to be $2a'$, which is the smallest distance, and systematically varying t_1 between $2a'$ and $6a'$ When looking at figure 5a we observe that as the parameter t_1 becomes larger we observe that the spectrum of many peaks for $t_1 = t_2 = 2a'$ and $t_1 = 3a'$, $t_2 = 2a'$ converges to a spectrum with a single peak for $t_1 = 4a'$, $t_2 = 2a'$ and higher. From this graph we conclude that the spectra $t_1 = 4a'$, $t_2 = 2a'$ and up are the closest to what we expect a topological boundary state to look like, because the single peak suggest a high concentration of electrons at the end of the chain, while the middle/bulk is nearly devoid of electrons. We will now investigate the configurations with $t_1 = 5a'$ more closely.

Now that we have decided on our first parameter to be $t_1 = 5a'$ we will take a closer look at what happens when we systematically alter the second parameter, t_2, from the smallest distance of $2a'$ to $5a'$. In figure 5b we can observe that if the value t_2 comes closer to t_1, we observe that the spectrum starts to show more peaks. The appearance of more peaks in the spectrum

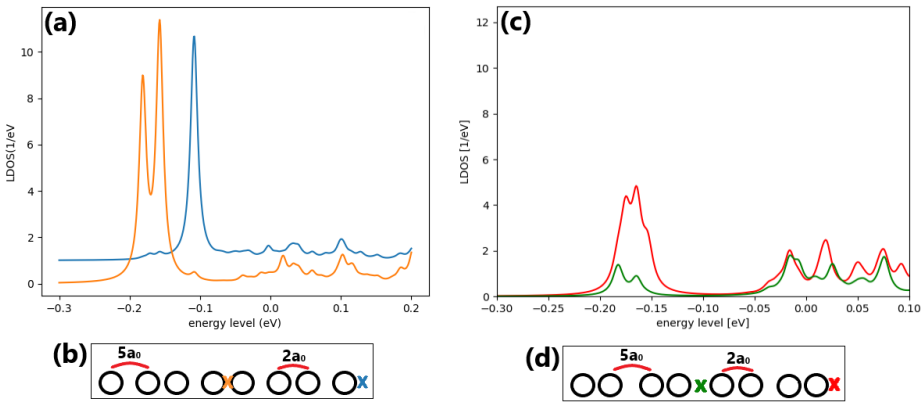

Figure 6: (a) The LDOS spectra for the parameters $t_1 = 5a'$ and $t_2 = 2a'$. The blue spectrum is taken at the end of the chain, the orange spectrum is taken at the middle of the chain. (b) A schematic depiction of the arti cial atoms with markings denoting the places where the spectra from gure 6a are taken. (c) The LDOS spectra for the parameters $t_1 = 2a'$ and $t_2 = 5a'$. The red spectrum is taken at the end of the chain, the green spectrum is taken at the middle of the chain. (d) A schematic depiction of the arti cial atoms with markings denoting the places where the spectra from gure 6c are taken.

means that the SSH chain loses the clear localization of electrons at the end of the chain. At $t_1 = 5a'$, $t_2 = 2a'$ we see the same spectrum as we saw in figure 5a. When we look at $t_2 = 3a'$, so t_2 becomes one step larger, we observe that the peak becomes less well defined. When we make t_2 another step larger we find that small peaks appear, and we observe that the tip of the largest peak has split. When looking at $t_1 = t_2 = 5a'$ we find that the spectrum does not exhibit a single clear peak, which is expected for the delocalised phase.

4.3 A closer look at $t_1 = 5a'$, $t_2 = 2a'$.

Now we have found a configuration for which we suspect a topological boundary state to be present it is time to take a closer look at the chain in order to confirm if our suspicion is correct. When we look at figure 6a we observe that the blue spectrum which is taken at the end of the non-trivial chain manifests one peak at an energy of -0.1eV. The orange spectrum taken at the middle of the non-trivial chain shows 2 peaks at the energies of -0.18eV and -0.15 eV. We see that the peaks in the orange spectrum and the peak in the blue spectrum do not coincide. This indicates that there is an energy at which the electrons are mostly located at the boundaries of the chain. When looking at

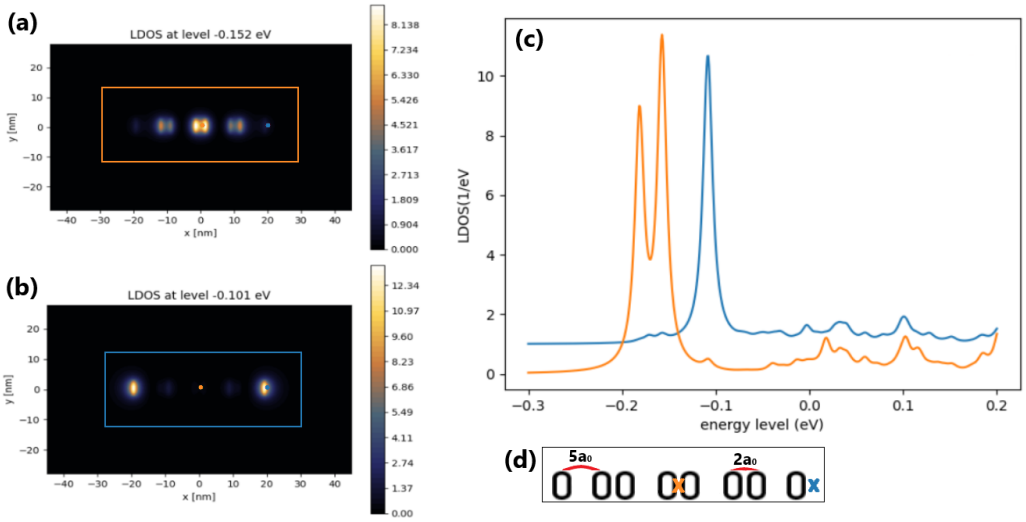

Figure 7: (a) The 2-dimensional LDOS taken at an energy of -0.152 eV. (b) The 2 dimensional LDOS taken at an energy of -0.101 eV. (c)The LDOS spectra for the parameters $t_1 = 5a'$ and $t_2 = 2a'$. The blue spectrum is taken at the end of the chain, the orange spectrum is taken at the middle of the chain. (d) A schematic depiction of the arti cial atoms with markings denoting the places where the spectra are taken.

figure 6c we observe that the spectrum of the trivial chain shows a bandgap between the conduction band and valence band. The bandgap in the orange spectrum from figure 6a is less well defined. When comparing figure 6a and 6c we note that the peak in the blue spectrum is located in the bandgap of figure 6c. We can also see that the peak in the blue spectrum is located in the bandgap of the orange spectrum. The bandgap in the orange spectrum is not well defined for these model parameters. Using other parameters, we can see a better defined bandgap. A figure showing this has been provided in the appendix. The presence of the blue peak in the bandgap is a good indication for the presence of a topological boundary state.

Now taking a closer look at the 2D LDOS maps for the non-trivial chain we observe in figure 7a that the orange peaks coincide with a high electron density around the centre artificial atoms. The electrons are not localized in this phase. When we look at figure 7b we can see that the single peak in the blue spectrum coincides with a high density of states at the ends of the chain. This is what we expect to find when a topological boundary state is present.

This behaviour is only manifested for the chain in this specific configuration. What happens when we switch around the parameters t_1 and t_2 such

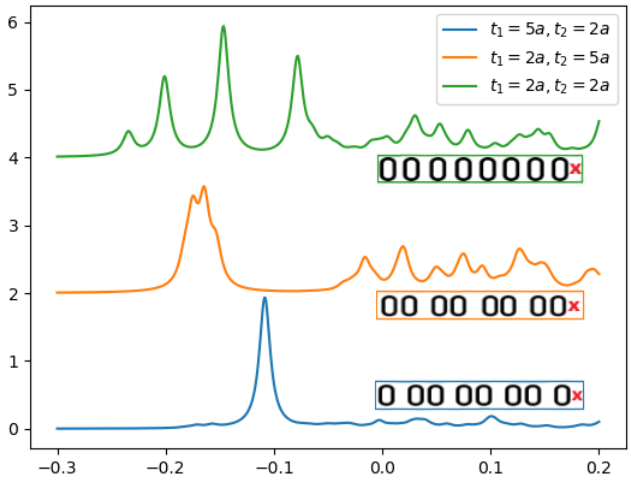

Figure 8: The LDOS spectra taken at the end of the chain for the delocalized chain with parameters $t_1 = t_2 = 2a'$ in green, the trivial chain with the parameters $t_1 = 2a'$ and $t_2 = 5a'$ in orange, and the nontrivial chain with parameters $t_1 = 5a'$ and $t_2 = 2a'$ in blue.

that $t_1 > t_2$? We find that this results in a trivial chain for which we do not observe a clear peak in the LDOS, this is shown by the orange line in figure 8. The green line in this figure is the spectrum of the chain for which $t_1 = t_2 = 2a'$, which is the delocalized variant of the chain.

Now that we have found clear evidence of a topological boundary state we can take a look at the influence of the physical properties of the chain on the manifestation of a topological boundary state. We will be taking a look at the influence of the size of the artificial atoms and the length of the chain on the peak in the spectrum taken at the end of the chain. Looking at figure 9a we can see the effect of the artificial atom's size on the manifestation of the peak. We observe that for artificial atoms comprising of 1 through 3 atoms each, we find that the spectrum does not manifest a clear peak. For the artificial atom sizes 4 through 6 we do observe a more clearly defined peak. The non-manifestation of the peak at the smaller artificial atom sizes can be explained by the lower coupling between the artificial atoms at lower artificial atom sizes. We also observe a shift in the location of the characteristic peak in the spectrum. The location of the peak shifts to a lower energy as the artificial atoms become larger, this is caused by the stronger coupling between the artificial atoms.

4.4 How many artificial atoms do we need?

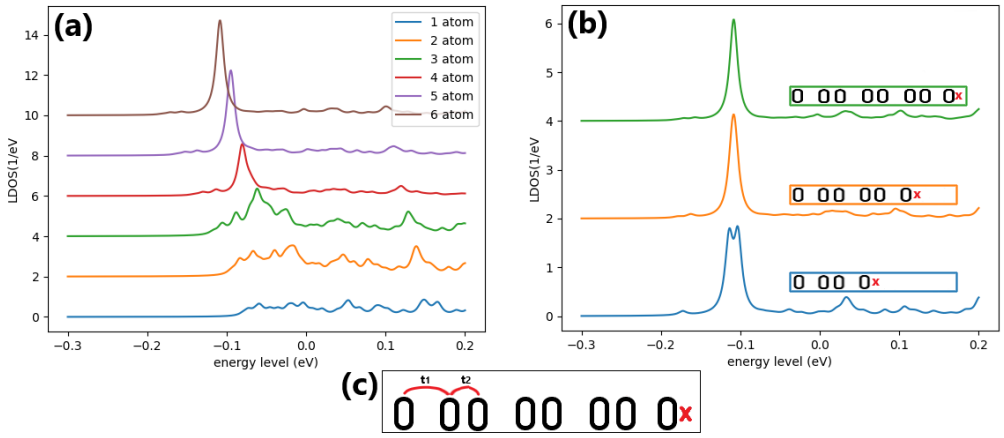

Figure 9: (a) The LDOS spectra for di erent size arti cial atoms using the parameters $t_1 = 4a'$ and $t_2 = 1a'$. (b) The LDOS spectra for a chain of 4, 6, and 8 arti cial atoms for the parameters $t_1 = 4a'$ and $t_2 = 1a'$. (c)A schematic depiction of the arti cial atoms with a red cross marking the position where the spectra in gure a are taken.

If we look at the effect of the chain length on the spectrum as shown in figure 9b, we observe that the spectrum of the non-trivial chain stays well defined for chain lengths of six and eight artificial atoms. For the four artificial atom chain, we observe that the spectrum does not manifest a well-defined peak, due to the tip being split. This less defined peak is still located at the same energy level of -0.1V as the peaks in the spectra for configurations comprised of more artificial atoms.

5 Conclusions and Outlook

With the results of the numerical simulations, we can make decisions on how to realize the SSH chain using an STM. We have found that the best way to construct an In SSH chain on an InAs(111)A platform is using artificial atoms made of 6 In atoms each to ensure that the coupling between the artificial atoms is optimal. The parameters that give the best result for a chain made of these artificial atoms are $t_1 = 5a'$ and $t_2 = 2a'$. The length of the chain must be at least 6 artificial atoms to find a well-defined peak in the energy spectrum at -0.1eV.
Future research could look into building this specific configuration in order to experimentally confirm the findings of this numerical simulation. Once our model is validated by experimental data, researchers could look at the feasibility of building a so-called higher-dimensional topological insulator such as a 2-D topological insulator.

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7 Appendix

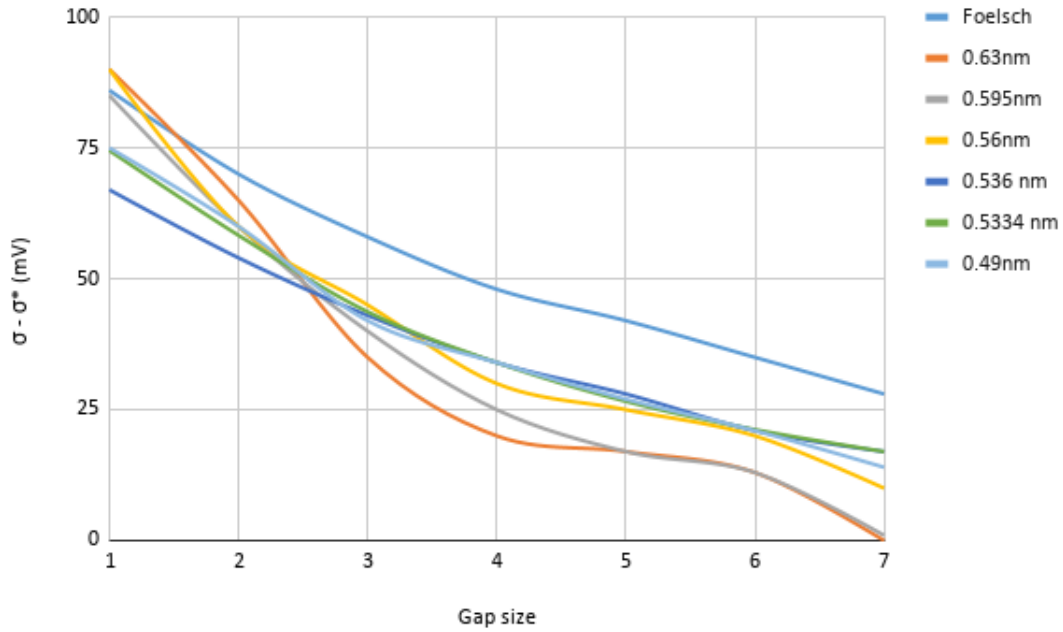

Figure 10: The $\sigma - \sigma*$ splitting as a function of gap size for di erent FWHM, with a gaussian height of -2.0eV.

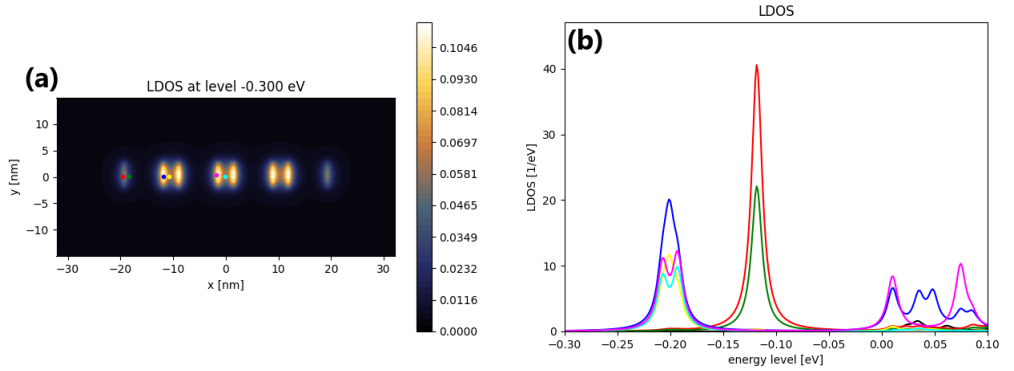

Figure 11: (a)A spacial LDOS of a SSH chain for a Gaussian height of -3.0eV and a FWHM of $0.6a'$ for the hopping parameters $t_1 = 5a'$ and $t_2 = 2a'$. The colored dots indicate the measurement locations of the similarly colored lines in gure 11b. (b)The LDOS taken at di erent locations. Notice that the peaks of the spectrum taken at the end of the chain lie within the band gap. (This image was provided to me by Thomas Gardenier).