LUCA MONTARELLI: Hello, everyone. Today I am going to talk to you about crystallographic point groups. And how to visualize them with Mathematica. Point groups are important in crystallography as they enable us to classify symmetries of crystals.

So what are point groups? Point groups are sets of symmetries which are invariant around the center point. Meaning a point will not change if it's at the center. And the has all of these symmetries applied. There are three elements of point groups. Mirror planes, rotation axis, and roto-inversion axis.

And mirror planes as we can imagine, are just taking a point. And then the mirror image of this point would be the symmetry. Mirror planes can be in three dimensions. Meaning that they can be perpendicular to x, perpendicular to y, and perpendicular to the z-axis.

Rotation axis are also found in the three dimensions. But they are rotations around this axis. So for example, a two-fold rotation would be taking a point and making a rotation of half a circle around a certain axis. And this would be the symmetry. A three-fold rotation axis would be three atoms which are each rotated by one third of a circle, so.

Roto-inversion axis are a bit more complicated to visualize, there are basically a rotation followed by what we called an inversion. So for example, if we take a full forward roto-inversion axis we have to take our point, rotate it by one fourth of a circle. And then invert this point through the origin. So basically inverting would be taking a point which has the coordinates one and one and transforming it into minus one, minus one, minus one.

When we mix all of these elements. we get the 32 point groups which are in crystallography as you can see in their 2D notation like this. So let's talk a bit about the notation. It is fairly simple.

We take an m if we have a mirror plane. Two m's if we have the two mirror planes et cetera. If this mirror plane is perpendicular to an already existing rotation axis then we note its slash m. A rotation axis is basically just a number which tells us the number of rotations. So three-fold rotation axis would be three rotation around a certain axis. Axis power is also denoted for a roto-inversion axis.

So if we look at examples, a couple of examples. We can see the first point group which is named one. Which basically has no symmetry. So we have a point and nothing happens with

it.

Then we have the two-fold rotation axis. So we take [INAUDIBLE] at this point, rotate it by half a circle, and we get this point. Same for the three-fold rotation axis. One, two, and three. And we are back to the original position. And then we have here the four-fold rotation axis. And here the six-fold rotation axis.

If it take something which has mirror planes, this is m, m, m. So for example, we can take the cross. Which the cross symbolizes an atom which is above the plane. And a circle an atom which is below the plane.

So if we take this point and then say that there is a mirror plane here. Then we have of course to find a mirror image which is here. Then if we say it is a mirror plane on this direction, then we have to take these two atoms and put them here.

And then we also have a third mirror plane which would be perpendicular to the x-axis. So the x-axis in these images goes out of the screen. And that's how we end up with four atoms on the top and four atoms below. And then we can combine these with a rotation axis.

So for example this is a two slash m. So basically we have a two-fold rotation. And then we have a mirror plane which is perpendicular to the x-axis. So we get two atoms above and two atoms below. You can also play around with the rest and see if it works.

But it gets more and more complicated up to this one, which is m bar three m, which is the most symmetric of these point groups. So how do we use point groups? Basically if we combine the 32 point groups with the translation symmetries of the 14 Bravais lattices. And glide plane's complex co-axis which are found in 3D. If you start to combine point groups then we end up with a 270 space group to which all crystals belong.

So how do we combine point groups and Bravais lattices? So here is a list of the Bravais lattices. They're basically just taking a point and translating it around cubic lattice, the trigonal lattice, hexagonal-- everything. The blue point will be the center of the point group. And then we just translate this mass of atoms which are the cemetry on the point group and then translate it around lattice.

So let's look at a code and see how we visualize that. So this is the manipulate, which has a function embed inside. So we start with one atom which is the point group one.

If we decide to make a mirror plane for example, perpendicular to x, then we end up with this. This is just one mirror plance which has the name one. Then plane m [INAUDIBLE]. Then we can have three mirror planes which would give us eight atoms. And this is basically what the code does. Just taking all of what we give it.

So for example we can take two, two, two which you can find is this one here. Two, two, two gives us this. So this is the two, two, two rotation axis. A symmetric two, two, two point group. Here in the function we also have the number of atoms, which is four. And we have the name of the point group which is a bit experimental because it's not easy to generate a name out of the [INAUDIBLE].

This code can generate-- for example this. Which is upon group which does not exist, six, six, six. This is a first version of the code which might be improved of course. We can also take roto-inversion axis here.

So if we try to understand what's happening with this one is we have an atom. So we set one for rotation. And rotoinversion axis would be a 1:4 rotation. So basically we end up at the same point. And then we inverted through the origin and then [? weak ?] this opposite atom, as you can see.

If we get things maybe clearer to see if we have the three rotoinversion axis. So here you can clearly see that the 3:4 rotation. So we have three atoms on one side and three atoms on the other side. So three atoms above and three atoms below. And then we invert them each time.

So this is the coding. Now let's look at how it works. So it is quite easy. What the code does is taking inputs and then calculating all the matrices of modal transformations. So the first line, here, would be taking the matrix to be replaced. So with the functional deflection transform from Mathematica, this line takes the rotation axis with the rotation transform function.

Then these lines calculate all the rotation and all the transformation matrices from each rotoinversion axis. As you can see, it's a bit more complicated to come up with.

And then taking all of these matrices, which are found in the lines of matrices [INAUDIBLE], matrices, plots and matrices in for a rotoinversion. We do the outer products of all of these matrices, so we get every possible combination of every possible symmetry. So we can have more of these put into symmetry positions. And then we're applying that to our initial position and we get all the symmetry positions.

Then we get into duplicates of symmetry position. We make sphere out of it, and then we display everything in a Graphics3D. This bit here is to generate the name of the bond group. As I said, experimental. And this bit here is to calculate the number of atoms we have.

So this is basically the function, which is not that complicated, as I said. And here is the results that we can have, as you can see. We can start combining everything and having your two bar and two bar and two bar and. And just play with it. This is why this is great, because we can actually visualize putting groups in 3D, instead of seeing them as these two different presentations.

So I hope you had a fun time. And thank you for your attention.