Foundations of Computational Materials Modelling
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The Space groups

Good afternoon everyone, so let us continue from where we left off, we were talking about the screw rotations, and we talked about additional translation based symmetry operators which can exist in 3 dimensions or for the space lattice. One is called as the glide reflection where you reflected about a plane then move it in a direction on in a direction parallel to the lattice vectors with the magnitude of usually half the lattice vectors. So, we saw different kinds of glide reflections that is possible.

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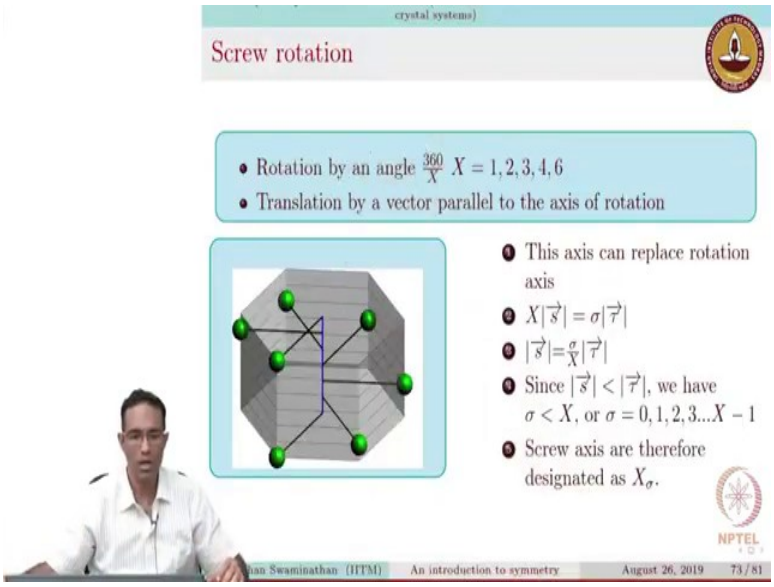

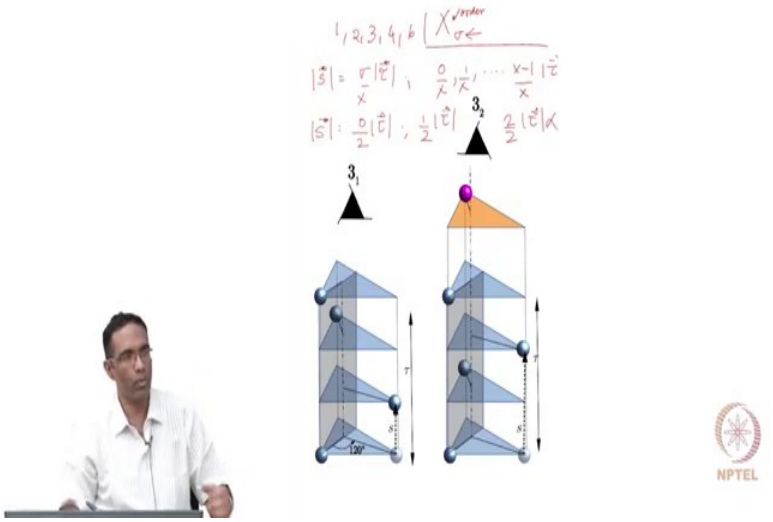

And we took an example of the orthorhombic system just to illustrate a couple of different glide reflections that is design actually possible. Then we went on to talk about the next translation based cemetery operations which is basically screw rotations and we took the example of 3, 1 and 3, 2, if you remember it correctly.

So, what happens in this particular operation is you perform a rotation one of the allowed rotations which is either 1 fold, 2 fold, 3 fold, 4 fold or 6 fold nothing else. And after performing this rotation you are able to move it by some amount in a direction along the along the axis of rotation.

So, we saw that, you know, you can basically perform this translation following the rotation by certain amounts, tau is basically the lattice vector and you can essentially have so many different types of translations possible following a rotation. For example, when we do the when we have 2 fold rotation, then the amount by which you can translate it will be 0 by 2 which is after rotation perform a full translation, which is basically nothing but a 2 fold rotation. Or you can have 1 over 2 times tau vector, which is essentially after performing a 2 fold rotation, you move it by half, the unit cell.

And then 2 over 2 times tau is not anything new, which is basically taking you back to the next cell, the same thing as 0. So, these are the various things possible and whenever you have such a symmetry operator present in the system, you label it with x suffix sigma. So, this will be the order of the rotation. And this sigma is essentially going to turn you by how much you are going to move this atom or whatever you want to move and by how much you want to move it, what fraction of the unit cell you want to move it.

So, this is what we did last class and we saw an example, which is 3 1 and 3 2. So, in 3 1 you took this atom, this was the atom and this entire thing is a unit cell, which is marked by tau. So, if there is an atom present here, there should be an atom that is also present here, perform a 3 fold rotation, move it by 1 over 3.

So, 3 suffix 1 means it is moved by 1 by 3 of tau that should be clear now. And then one more, 3 fold rotation, move it by one by three of tau, 1 more 3 fold rotation move it by 1 by 3 of tau. This entire thing is 1 unit cell. And if you repeat it in that direction, it is consistent with the lattice translations. Therefore, this is a correctly done 3 fold, 3, 1 screw axis. If you should take the three to screw axis, certain strange things begin to happen. You perform a rotation by 120 degrees and then do two thirds.

So, the amount by which you need to move can simply be obtained by looking at the symbol. Yes, there is a question yes, 3 1 is same as, not 3 1 by 3 fold rotation, plus and followed by one third of the unit cell. So, if this is the symbol for the screw rotation, that means, after performing a rotation of order x, I perform a translation by sigma by x times tau. So, just by looking at the symbol, you know that the x goes to the denominator and sigma goes to the numerator. So, 3 1 means one third of the translation, 3 2 means two third of the translation of the unit cell vector.

So, when you perform 3, 2, you move it by 120 degrees, we are looking at we are studying 3 2 now, move it by 120 degrees, rotate it by 120 degrees, and move two thirds of the unit cell. This entire thing is actually the unit cell. So, you are moving two thirds of the unit cell. So, first, the atom ends up here, then you have to keep performing these operations and they have to keep lying on top of each other. That is the whole spirit of symmetry.

So, let us perform this operation on this atom that we just generated. You perform 120 degree rotation and then move it up. It ends up in this spot, which is actually the next unit cell is not in the same units cell. But you can understand that if there is an atom here, there should be an atom here by translation. And this layer is the first layer that is on top of this base layer of the second unit cell, which means there must be an atom even here.

So, now you perform the 120 degree rotation and the translation for this system, 120 degree rotation and then 2 by 3, it ends up right here. So, the, these 4 atoms are to be generated when you perform 3 2 screw rotation symmetry. And I highlighted that if you put a mirror like that, then this atom is going to stay right there because it is present on the mirror.

However, this atom is possible that it can reflect it to this spot right here. This atom can get reflected to this spot right here. And this atom does not get affected at all, which is basically 3 2 two. If you put a mirror plane and look at where the atoms are generated, it will look very similar to what was generated with 3, 2.

Consequently, 3 1 and 3 2 are essentially mirror images of each they are called as enantiomorphous pairs. There are some interesting physical consequences because of the presence of this symmetry. So, we will not be discussing that in this class.

The symbols for these screw rotation axis is also important. So, you have a triangle followed by these extensions, which is basically the symbol for the screw rotation. And if you look at 3, 1, it is as good as it is rotating in the counterclockwise direction, whereas 3 2, it is as if it is rotating in the clockwise direction essentially telling you that they are mirror images or enantiomorphous pairs. So, this is what we saw last class.

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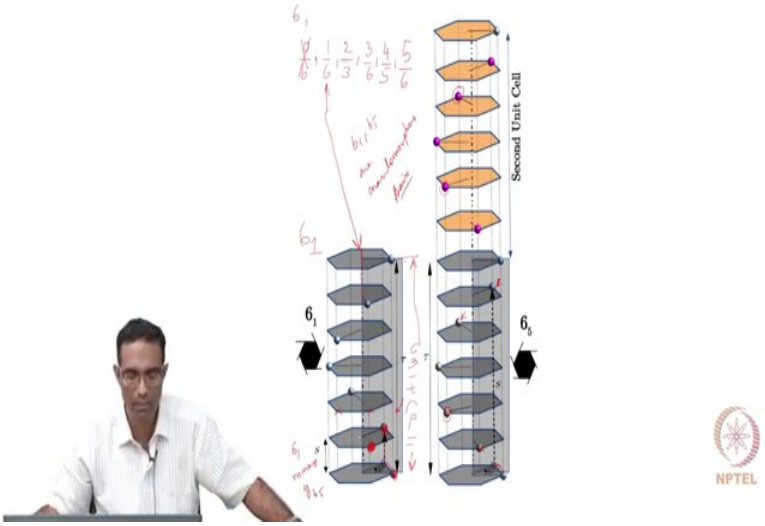

And I wanted to show you a couple of more examples especially with 6, 1 and 6, when you have 6 rotations that is when you have the 6 fold rotation possible. When you have 6 fold rotation possible, several translations are possible. So, translations that are possible are 0 by 6, which is not very interesting to study. But you have 1 by 6, 2 by 6, 3 by 6, 4 by 6 and 5 by 6.

So, in this image right here, I have, after performing the 6 fold rotation, I have moved it one sixth of the unit cell and that fold is called a 6 1 axis. So, this is called a 6 1 axis. So, what is happening here?

You have the atom present at this part. I am going to perform a 60 degree rotation, which is basically a 6 fold rotation. And then I am moving it one sixth of the unit cell.

So, the entire unit cell is, this is the entire unit cell. This is the entire unit cell, I am moving at one sixth of the entire unit cell. So, 1, 2, 3, 4, 5, 6, we have performed the 6 times. I will essentially make this atom land up here. And if I repeat this in the direction of the axis of rotation, I will essentially be performing lattice translations and it all looks like one big spiral staircase going on right as you keep rotating.

And after every unit, at every unit cell, you will have this atom and this atom coinciding, which is what we want, correct, they should all be commensurate with lattice translations. This is 6 1. Now, what happens when you perform 6 5? We want to study 6 5 because I want to show you the corresponding enantiomorphous pairs. When you perform 6 5, you rotate it by 60 degrees, but now, you do not move it by 1 by 6, but you move by five sixth of the unit cell. So, 5, 6 of the unit cell will make this rotated atom, land up in this part right here, correct?

Perform and move, it we make it land up here. So, at this point, it appears as if when we perform these operations, nothing is going to be present in these intermediate planes. But that is not true. We will see that all those planes also get filled up. Now, you perform one more round of 6 fold rotation and 5 by 6 the translation. So, you move this here and then move it five sixth of the unit cell. So, 1, 2, 3, 4, 5, sorry 2, 3, 4, 5, it ends up right here, correct? Now the question is this is present in the next unit cell.

Now, how do we pull it back to our original unit cell, whereas the atom present in our original first unit cell? So, that is not very hard. So, this was the base, this is the base. So, this is the 1, 2, 3, fourth plane or 4 by sixth of the unit cell that this atom is present, since they should be commensurate with lattice translations. We should also have an atom at the exact same position, 4 layers above our initial first unit cell. So, 1, 2, 3, 4 right here, it ends up right here. So, this atom is the same as this atom.

Now, you perform one more 60 degree rotation and 5 by sixth of the distance. So, bring this here, 1, 2, 3, 4 comes here, but that is actually 1, 2. 2 planes above the base plane, so 1, 2, which means there should be an atom right here. You keep doing this over and over again. You will figure out that all these planes are also going to be filled up by atoms.

Now, you put a plane mirror like that and try to see where the atoms are getting reflected because of the presence of the plane. So, this atom again will not get reflected, but this atom will get reflected here, this is going through the center. It is going to the center of this hexagonal pyramid.

So, this will this atom will get reflected here because of this plane, which is nothing but this atom and this atom will get reflected here, sorry will get reflected here which is nothing but the third one this atom and so on. So, you will see that the atoms are getting reflected because of this plane and 6, 1 is nothing but a mirror image of 6, 5. And that is a plane through the plane that is passing through those, the plane that is passing right through the center of this hexagonal pyramid.

Similarly, 6 5, if you put a plane a mirror right there, and look at where the atoms are getting reflected, you will see that it is nothing but a mirror image of 6 1. So, 6 1 and 6 5, are enantiomorphous pairs again. You are able to see it?

Student: cursor movement is not visible.

Professor: Which one? I am sorry, you are not able to see the cursor moving, the point moving. So, what was not clear can I repeat it? Is there anything that was not clear? Is okay, are able to understand which atom is getting reflected because of this plane where and why 6 1 one and 6 5, turn out to be mirror images of each other? Yes, I will be careful from henceforth.

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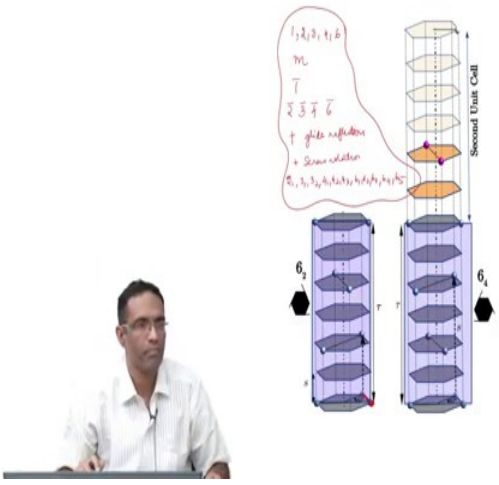

So, the next thing, next example is 6 2 and 6 4. As you can imagine, they are also enantiomorphous pairs. So, but in this case, slightly strange things will happen. So, it will tell you, you know, how the molecule should actually look. So, if you take the, you should take this atom and rotate it by 60 degree, you not able to see anything there . So, if I take this atom and rotate it by 60 degree and move it by two sixth, or one third of the unit cell, it ends up here. Now, I perform the operation again, ends up here, it ends up here.

So, because this is a unit cell there is an atom at this position? There should be an atom at this position. But by performing the 6 2 operation, a certain number of times I ended up with an atom right here, which means there has to be an atom in this spot as well.

Consequently, all these planes get additional atoms and, you know, this is the way the 6 2 rotations look, 6 4 rotation is also similar except that now you will generate one in the unit cell that is above it. But you all know now, how to bring it back into the unit cell by properly examining what Basel plane it is located at and then pulling it back into the initial unit cell. So, these are the kind of operations which is permitted by your screw rotation.

So, the presence of 1 fold rotation, so all the operations if you look at once again, so 1, 2, 3, 4, 6 for all the rotations possible. The mirror planes, the inversion center, 2 bar, 3 bar, 4 bar, 6 bar plus glide reflections plus screw rotations which are nothing but 2 1, 3 1, 3 2, 4 1, 4 2, 4 3, 6 1, 6 2, 6 3, 6 4 and 6 5.

If you combine all the set of operations and examine the total number of possible ways you can arrange points in 3 D space, you will get 230 different ways possible and they are referred to as a 230 space groups. So, we will now look at these space groups and what they are and how they are classified.

But before doing that, do you have any questions? With regards to the screw rotation, there are a couple of things that I have not done. For example, 4 1, 4 2, 4 3 you should try it out in your, you know at home and try to convince yourself that even those contains some enantiomorphous pairs, so on and so forth. Yes, you had a question?

Student: Sir about the rotation. How it happens.

Professor: Rotation of screw rotation?

Student: So, 6 1, 6 4.

Professor: Yes.

Student: So, we see it is kind of opposite opposite, so we can take 6 2 as that one only.

Professor: You mean to say, if one is this, the other one is the other way. I think it is better to look at it that way. You are saying that I would have looked rotated this one anticlockwise, call it 6 2 and rotated that as that clockwise and call it 6 4. Yes, it is possible but that is why I have put them in pairs. If you have 6 2 you represented, this way then 6 4 is represented in the in a manner that is mirror image of this.

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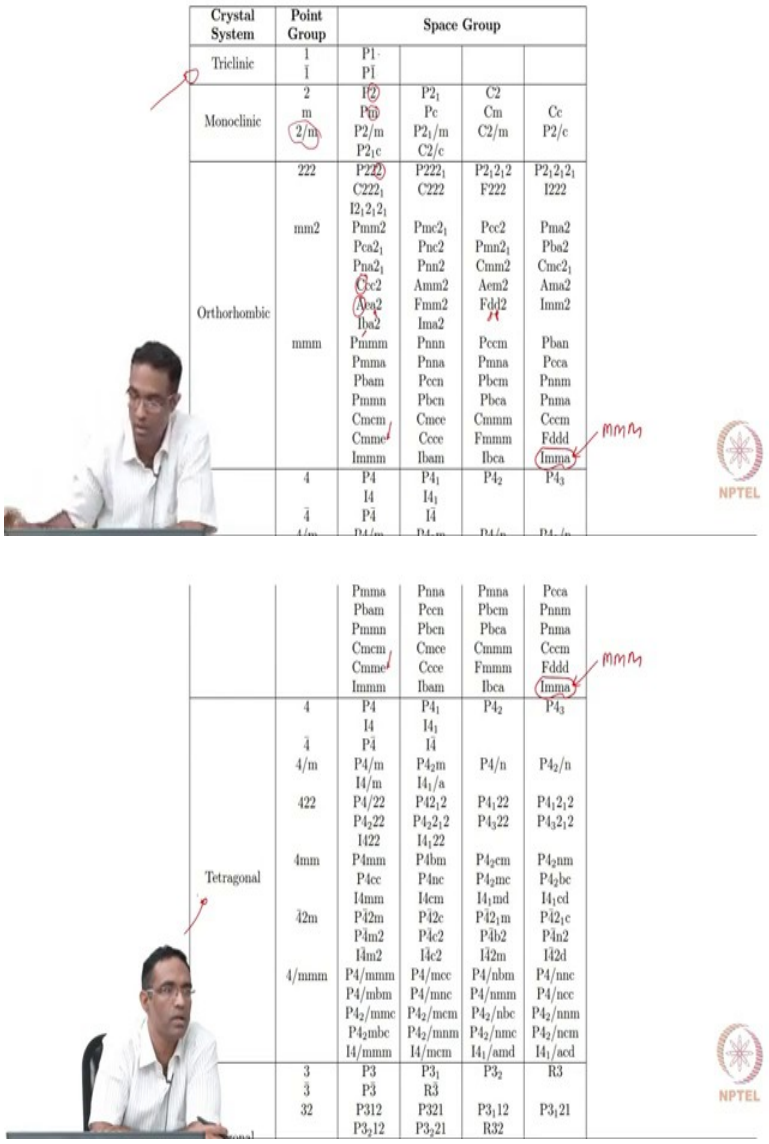


Crystal System	Point Group	Space Group			
Triclinic	1	P1			
	$\bar{1}$	$P\bar{1}$			
Monoclinic	2	$P2$	$P2_1$	C2	
	m	Pm	Pc	Cm	Cc
	2/m	P2/m	$P2_1/m$	C2/m	P2/c
		$P2_1/c$	C2/c		
Orthorhombic	222	P222	$P222_1$	$P2_12_12$	$P2_12_12_1$
		$C222_1$	C222	F222	I222
		$I2_12_12_1$			
	mm2	Pmm2	$Pmc2_1$	Pcc2	Pma2
		$Pca2_1$	Pnc2	$Pmn2_1$	Pba2
		$Pna2_1$	Pnn2	Cmm2	$Cmc2_1$
		Pcc2	Amm2	Aem2	Ama2
		Aea2	Fmm2	Fdd2	Imm2
		Iba2	Ima2		
	mmm	Pmmm	Pnnn	Pccm	Pban
		Pmma	Pnna	Pmna	Pcca
		Pbam	Pccn	Pbcm	Pnnm
		Pmmn	Pbcn	Pbca	Pnma
		Cmcm	Cmce	Cmmm	Cccm
		Cmme	Ccce	Fmmm	Fddd
		Immm	Ibam	Ibca	Imma
Tetragonal	4	P4	$P4_1$	$P4_2$	$P4_3$
		I4	$I4_1$		
	$\bar{4}$	$P\bar{4}$	$I\bar{4}$		
	4/m	P4/m	$P4_2m$	P4/n	$P4_2/n$
		I4/m	$I4_1/a$		
	422	P422	$P42_12$	$P4_122$	$P4_12_12$
		$P4_222$	$P4_22_12$	$P4_322$	$P4_32_12$
		I422	$I4_122$		
	4mm	P4mm	P4bm	$P4_2cm$	$P4_2nm$
		P4cc	P4nc	$P4_2mc$	$P4_2bc$
		I4mm	I4cm	$I4_1md$	$I4_1cd$
	$\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2c$	$P\bar{4}2_1m$	$P\bar{4}2_1c$
		$P\bar{4}m2$	$P\bar{4}c2$	$P\bar{4}b2$	$P\bar{4}n2$
		$I\bar{4}m2$	$I\bar{4}c2$	$I\bar{4}2m$	$I\bar{4}2d$
	4/mmm	P4/mmm	P4/mcc	P4/nbm	P4/nnc
		P4/mbm	P4/mnc	P4/nmm	P4/ncc
		$P4_2/mmc$	$P4_2/mcm$	$P4_2/nbc$	$P4_2/nnm$
		$P4_2mbc$	$P4_2/mnm$	$P4_2/nmc$	$P4_2/ncm$
		I4/mmm	I4/mcm	$I4_1/amd$	$I4_1/acd$
Trigonal	3	P3	$P3_1$	$P3_2$	R3
	$\bar{3}$	$P\bar{3}$	$R\bar{3}$		
	32	P312	P321	$P3_112$	$P3_121$
		$P3_212$	$P3_221$	R32	

		I4mm	I4cm	$I4_1md$	$I4_1cd$
	$\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2c$	$P\bar{4}2_1m$	$P\bar{4}2_1c$
		$P\bar{4}m2$	$P\bar{4}c2$	$P\bar{4}b2$	$P\bar{4}n2$
		$I\bar{4}m2$	$I\bar{4}c2$	$I\bar{4}2m$	$I\bar{4}2d$
	4/mmm	P4/mmm	P4/mcc	P4/nbm	P4/nnc
		P4/mbm	P4/mnc	P4/nmm	P4/ncc
		$P4_2/mmc$	$P4_2/mcm$	$P4_2/nbc$	$P4_2/nnm$
		$P4_2mbc$	$P4_2/mnm$	$P4_2/nmc$	$P4_2/ncm$
		I4/mmm	I4/mcm	$I4_1/amd$	$I4_1/acd$
Trigonal	3	P3	$P3_1$	$P3_2$	R3
	$\bar{3}$	$P\bar{3}$	$R\bar{3}$		
	32	P312	P321	$P3_112$	$P3_121$
		$P3_212$	$P3_221$	R32	
	3m	P3m1	P31m	P3c1	P31c
		R3m	R3c		
	$\bar{3}m$	$P\bar{3}1m$	$P\bar{3}1c$	$P\bar{3}m1$	$P\bar{3}c1$
		$R\bar{3}m$	$R\bar{3}c$		
Hexagonal	6	P6	$P6_1$	$P6_5$	$P6_2$
		$P6_4$	$P6_3$		
	$\bar{6}$	$P\bar{6}$			
	6/m	P6/m	$P6_3/m$		
	622	P622	$P6_122$	$P6_522$	$P6_222$
		$P6_422$	$P6_322$		
	6mm	P6mm	P6cc	$P6_3cm$	$P6_3mc$
	$\bar{6}m2$	$P\bar{6}m2$	$P\bar{6}c2$	$P\bar{6}2m$	$P\bar{6}2c$
	6/mmm	P6/mmm	P6/mcc	$P6_3/mcm$	$P6_3/mmc$

System	Group	Space Group			
Cubic	23	P23	F23	I23	$P2_13$
		$I2_13$			
	$m\bar{3}$	$Pm\bar{3}$	$Pn\bar{3}$	$Fm\bar{3}$	$Fd\bar{3}$
		$Im\bar{3}$	$Pa\bar{3}$	$Ia\bar{3}$	
	432	P432	$P4_232$	F432	$F4_132$
		I432	$P4_332$	$P4_132$	$I4_132$
	$\bar{4}3m$	P43m	F43m	I43m	P43n
		F43c	I43d		
	$m\bar{3}m$	Pm3m	Pn3n	Pm3m	Pn3m
		Fm3m	Fm3c	Fd3m	Fd3c
		Im3m	Ia3d		

Table 1: Space Groups and their Hermann-Maugin symbols

1 Introduction

In the following, the simple (non-primitive) lattice vectors based unit cell, which are generally used to construct the crystals are given. The Wyckoff positions are also given for this setting in the website pbc. Note that, a, b and c are the lengths of the unit cell dimensions which is usually given or known and may be obtained from the website https://materialsproject.org/ as well. Furthermore, the angles α is between $\vec{b}$ and $\vec{c}$, β is between $\vec{a}$ and $\vec{c}$, while γ is between $\vec{a}$ and $\vec{b}$. Note that $\vec{a}$, $\vec{b}$ and $\vec{c}$ are vectors given in the cartesian coordinate system.

2 Lattice vectors

2.1 Triclinic

$$\vec{a} = a\hat{i} \tag{1}$$

$$\vec{b} = b\cos(\gamma)\hat{i} + b\sin(\gamma)\hat{j} \tag{2}$$

$$\vec{c} = c_x\hat{i} + c_y\hat{j} + c_z\hat{k} \tag{3}$$

$$c_x = c\cos(\beta) \tag{4}$$

$$c_y = \frac{c(\cos(\alpha) - \cos(\beta)\cos(\gamma))}{\sin(\gamma)} \tag{5}$$

$$c_z = \sqrt{c^2 - c_x^2 - c_y^2} \tag{6}$$

2.2 Monoclinic

It is usually given such that the $\vec{b}$ direction is the unique axis. Which means, the $\vec{b}$ is the 2- fold rotation axis

$$\vec{a} = a\hat{i} \tag{7}$$

$$\vec{b} = b\hat{j} \tag{8}$$

$$\vec{c} = c\cos(\beta)\hat{i} + c\sin\beta\hat{k} \tag{9}$$

2.3 Orthorhombic

$$\vec{a} = a\hat{i} \tag{10}$$

$$\vec{b} = b\hat{j} \tag{11}$$

$$\vec{c} = c\hat{k} \tag{12}$$

2.4 Tetragonal

$$\vec{a} = a\hat{i} \tag{13}$$

$$\vec{b} = a\hat{j} \tag{14}$$

$$\vec{c} = c\hat{k} \tag{15}$$

2.5 Hexagonal

$$\vec{a} = \frac{1}{2}a\hat{i} - \frac{\sqrt{3}}{2}a\hat{j} \tag{16}$$

$$\vec{b} = \frac{1}{2}a\hat{i} + \frac{\sqrt{3}}{2}a\hat{j} \tag{17}$$

$$\vec{c} = c\hat{k} \tag{18}$$

So, I prepared a sheet, we will be sharing that with you. So, now we are kind of getting to the point where we will be able to generate this crystal structures using our MATLAB script. But it is important for us to know what lattice vectors to choose depending upon the unit cell that is appropriate for that particular space group which are listed in this document.

I will also introduce you to a new website which is called as materials project dot org which is extremely useful for us to check several things that we check several things that we can after we construct the crystal structures, we may want to check a few things, so all these checking's can be done using this website materials project dot org. I will introduce you to that.

So, for all these units cells, triclinic, monoclinic, orthorhombic, tetragonal, hexagonal, trigonal rhombohedral and cubic, I have given down the lattice vectors there is most commonly used for generating the crystal structures. Mostly you will, it will be quite obvious what needs to be chosen, what needs to be your A vector, what needs to be B vector and what needs to be a C vector.

Sometimes it can be a little bit tricky, you have to read the notations carefully. You have to understand what the author of the paper that you are reading is using as a B vector or a C vector and based on that modify some of these statements a little bit to generate the crystal structures.

So, we will come to that later. But now, I want to look at these 230 space groups, so I have written on all the 230 space groups over here and classified the unit cells or the crystal system that is appropriate in order for you to generate the crystals belonging to each of these space groups.

So, like we discussed, if you have P1 one bar that means the only symmetry that is possible is either 1 fold rotation or maybe an inversion, if it is an inversion, it is basically the triclinic bravais lattice, right? Then you have to use a triclinic unit cell and correspondingly you will choose these as your, these as your lattice vectors and if you look at mono clinic, you will see nothing but a 2 fold rotation and a mirror. There is no other term that is present in the other slots. Yes.

Student: Zoom this.

Professor: You want me to zoom this also. Is this fine? So, the mono clinical lattice does not have anything other than a 2 fold rotation associated with it. So, if you look at the space groups, you only have 2, what was the monoclinic bravais lattice space group? It is just P 2 m. There is nothing as you had a 2 fold rotation and then a mirror plane is perpendicular to it.

So, if you have a 2 fold rotation and a mirror and nothing else, nothing else no other slots are filled here, then you will know that it is actually a mono, this actually need not be given to you at all from what we have discussed so far, just by looking at the space group, you should be able to identify what unit cell is appropriate to generate this crystal structure.

P 222 or P mmm or combination of 2 and m, combination of screw rotation in one of them, but not in the others, all these things are nothing but orthorhombic. Screw rotations will always be present whenever you have whenever a 2 whenever a rotation of that particular fold is possible.

Similarly, glide planes are going to be present whenever a mirror is possible in that particular location, you cannot have any other means. So, what is the point group corresponding to I mma? Point group, mmm that is it. That is the point group, you just remove all translation based symmetry operations.

So, you have a huge number of possibilities in the orthorhombic system. You will see some, you have we have seen the A glide, we have some B glides, we have seen some D glides, we have also seen, we have seen examples of D glides in one of our slides there. We have not seen examples of E glides which are also possible. I will let you figure out what that is. Then, in the orthorhombic space group, you have A centered which means our atom is going to be present in the A, in the plane which has the A axis as in normal.

You can also have atoms that is being centered about the C plane which means there is a there is an atom that is centered about the plane which has the C axis as a normal and so on. So, that is the orthorhombic space group then you have the tetragonal space group. So, you will have a combination of 4 fold rotation, the first one that will tell you the tetragonal is that there is a 4 fold rotation and then the next subsequent slots, you will either have nothing or you will have mirrors or 2 fold rotations and nothing else.

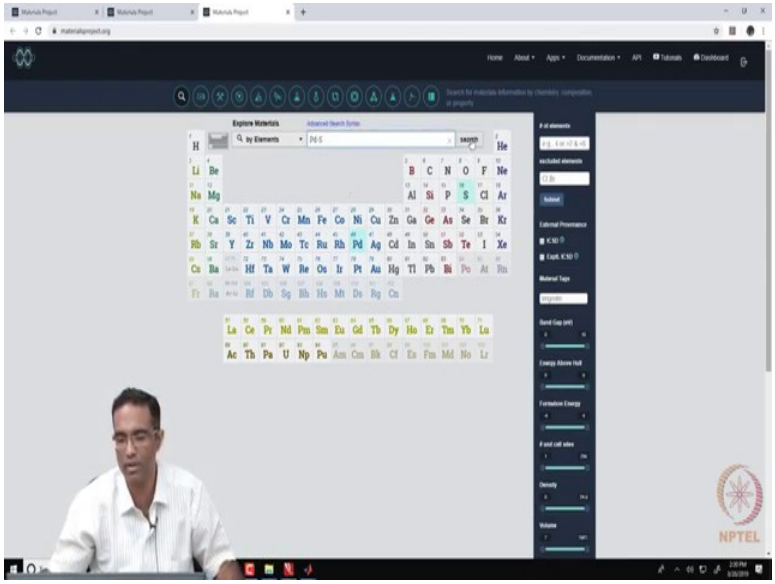
So, that will essentially give you a combination of several space groups which belong to the tetragonal which for which the tetragonal unit cell or tetragonal crystal system can be used. Then the trigonal is going to have 3 fold rotation in the first part and then followed by mirrors

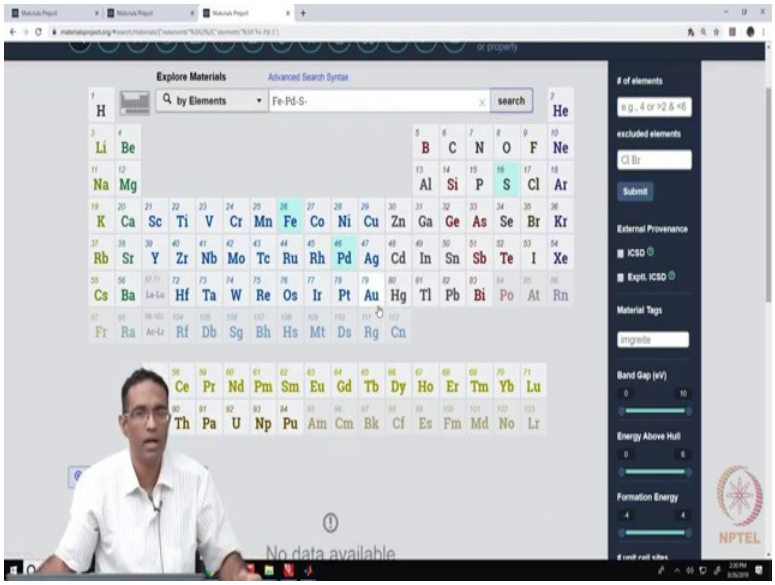
or nothing. If there is a 3 fold rotation obviously, it means you are providing, you know, additional symmetry operators such as 3 fold rotation with some screw axis being present that is also possible.

So, all these things are listed here, then you have the hexagonal system which should be very clear because of the presence of the 6 fold rotation. Then last you have cubic, the cubic is identified by the presence of 3 in the second slot, I mean second slot after this P or I. So, always you will have 3 or 3 bar that is been present. The first one will ever be a 4 fold rotation or a mirror or 2 fold rotation. You can take a look at it carefully and you will see that nothing else is present here.

So, people have already performed this classification. So, any crustal structure that you want to generate now, a proper crystal that you want to generate will actually be in one of these 230 space groups. So, we will now look at how we can actually look at some of the materials and the corresponding space groups. One of the websites that I found extremely interesting is this website called is the materials projects dot org.

(Refer Slide Time: 26:21)

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Advanced Search Syntax
by Elements
Fe-Pd-S-
search
# of elements
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Submit
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Material Tags
Band Gap (eV)
Energy Above Hull
Formation Energy
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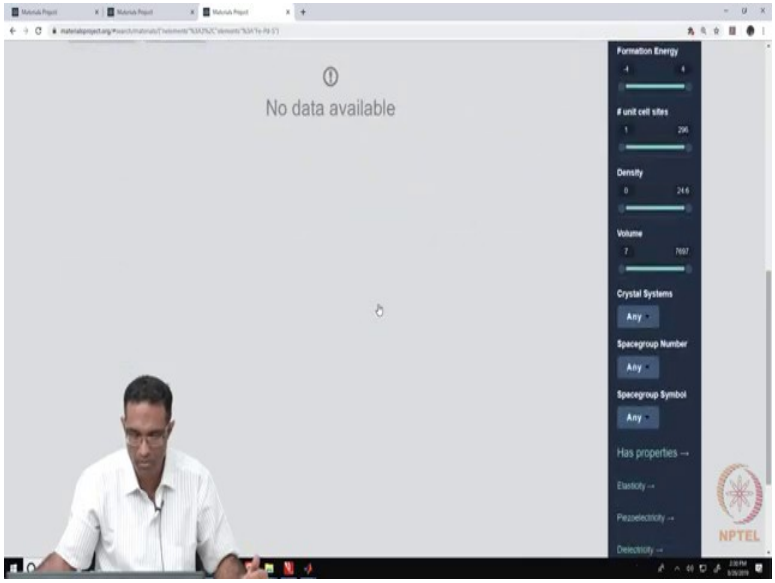
NPTEL


Formation Energy
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Spacegroup Symbol
Has properties →
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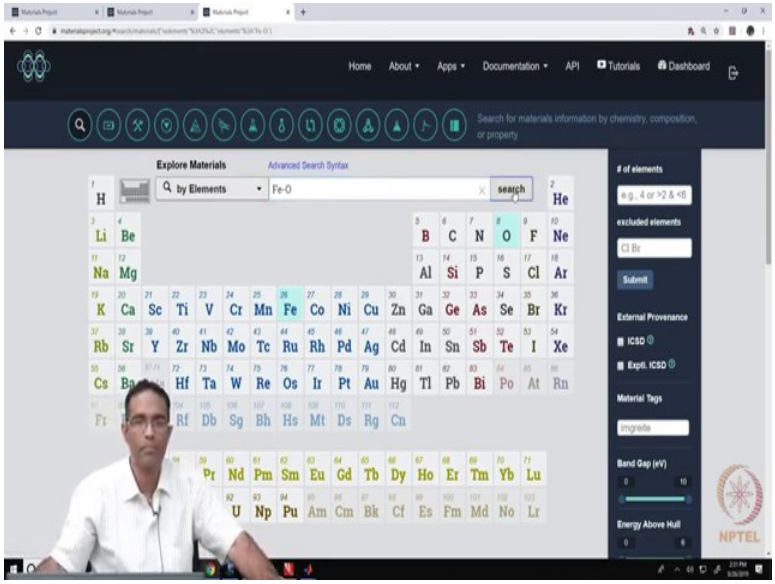
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by Elements
Fe-O
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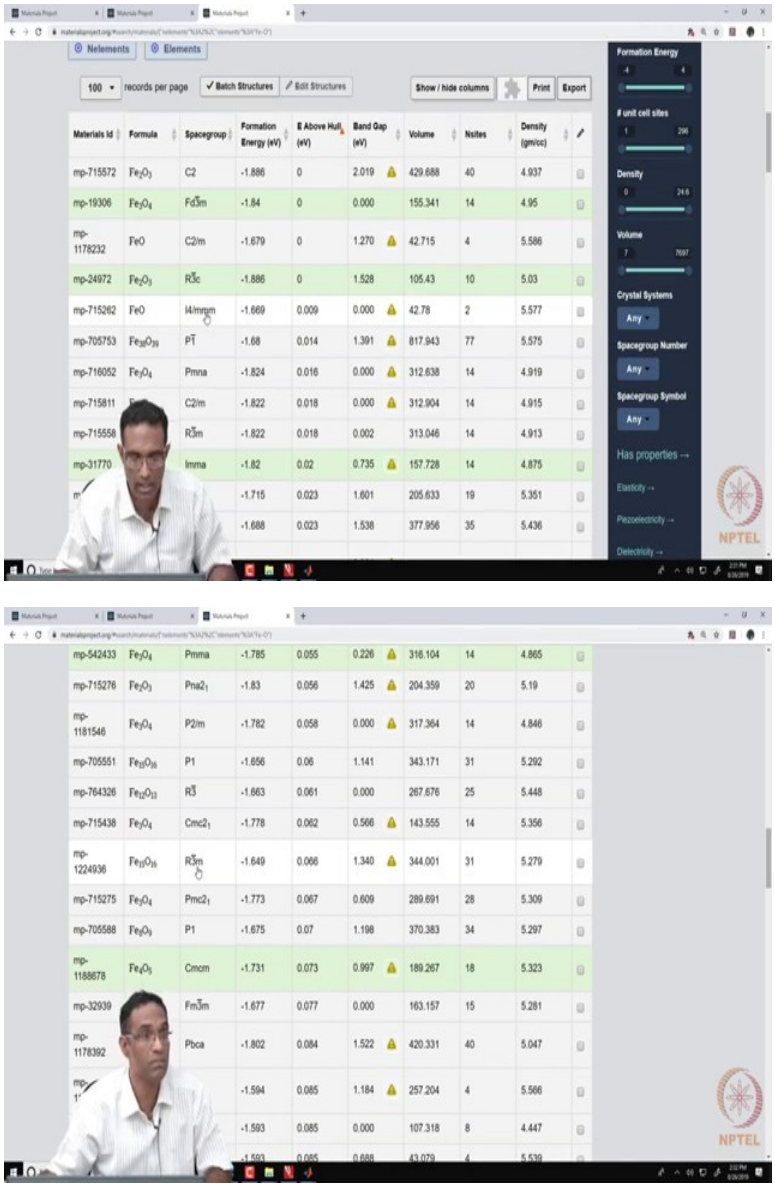


I think some of you may already be familiar with this website. If you are not, you can go and explore it is really amazing. So, you have to first create login and sign up. After you since I have already signed up here with my Google account, it is opening up my, it is opening up is opening up for me. So, now I can do lots of results, lots of research based on the kind of based on the structure that I want to read. Now, this course is focusing only on structure per se, we are not looking at other properties or thermodynamic properties of the material.

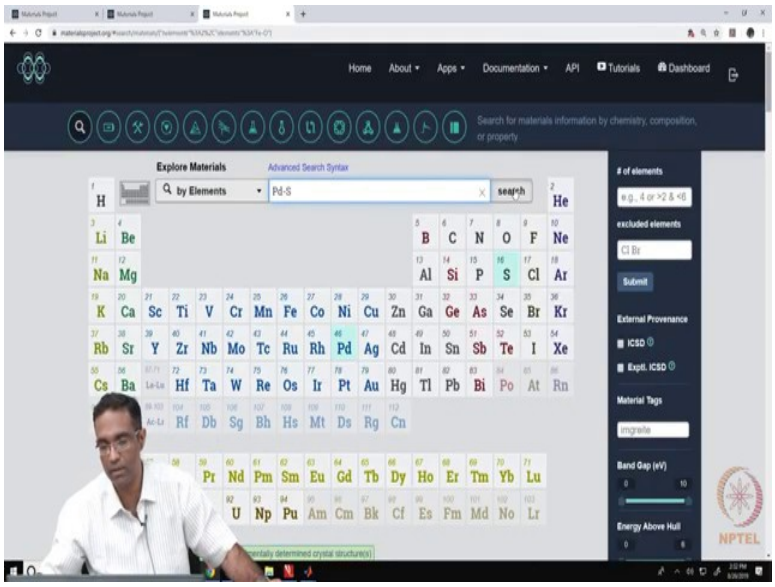
So, those things will, those things are irrelevant to us from this website, we will only look at these crystal structures. So, suppose I want to find what possible space groups are possible with the material, say palladium and cell phone, what possible space groups are possible? So, I just put these things here, I just put the 2 elements right here, followed by a hyphen, and click search. And it gives me all possible, so you get the periodic table. And you can, of

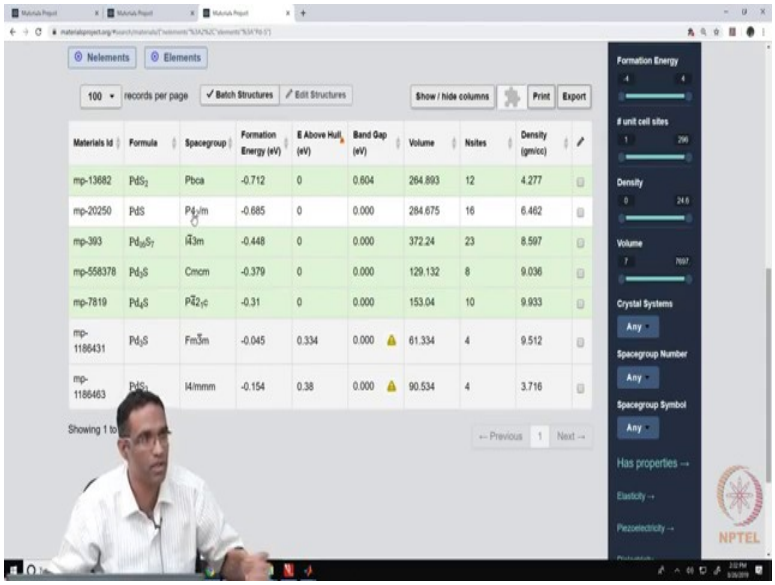
course, click on all these things to make stuff appear here. So, for example, once I click Iron, clicked Iron, it showed me Iron there.

So, if I did this and click search, it is going to tell me if there are compounds with iron, palladium and sulphur, no data available. So, nobody has found anything with these things, but let us look at our famous FeO and see what all turns up, you have huge number of a FeO compounds, huge number of a FeO compounds, showing 1 to 112 entries. So, basically, it runs to the next page as well right here. And so these are our components possible. This is the material's ID that these people have given to these compounds.

And the third column, we have our favorite space group for each of these compounds, each of these compounds you have the space group. So, if you look at FeO, it is I4 over mmm. So, can you tell me what unit cell you would use to generate that structure? Tetragonal, so you can keep going on and on. There is also a $Fe_{15}O_{16}$ with some rhombohedral space group several others.

(Refer Slide Time: 28:47)

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Elements
100 records per page
Batch Structures
Edit Structures
Show / hide columns
Print
Export
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mp-20250 | PdS | $P4_2/m$ | -0.685 | 0 | 0.000 | 284.675 | 16 | 6.462
mp-393 | $Pd_{16}S_7$ | $I\bar{4}3m$ | -0.448 | 0 | 0.000 | 372.24 | 23 | 8.597
mp-558378 | Pd_3S | Cmcm | -0.379 | 0 | 0.000 | 129.132 | 8 | 9.036
mp-7819 | Pd_4S | $P\bar{4}2_1c$ | -0.31 | 0 | 0.000 | 153.04 | 10 | 9.933
mp-1186431 | Pd_3S | $Fm\bar{3}m$ | -0.045 | 0.334 | 0.000 | 61.334 | 4 | 9.512
mp-1186463 | PdS_2 | I4/mmm | -0.154 | 0.38 | 0.000 | 90.534 | 4 | 3.716
Showing 1 to
← Previous 1 Next →
Formation Energy
unit cell sites
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Volume
Crystal Systems
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Spacegroup Symbol
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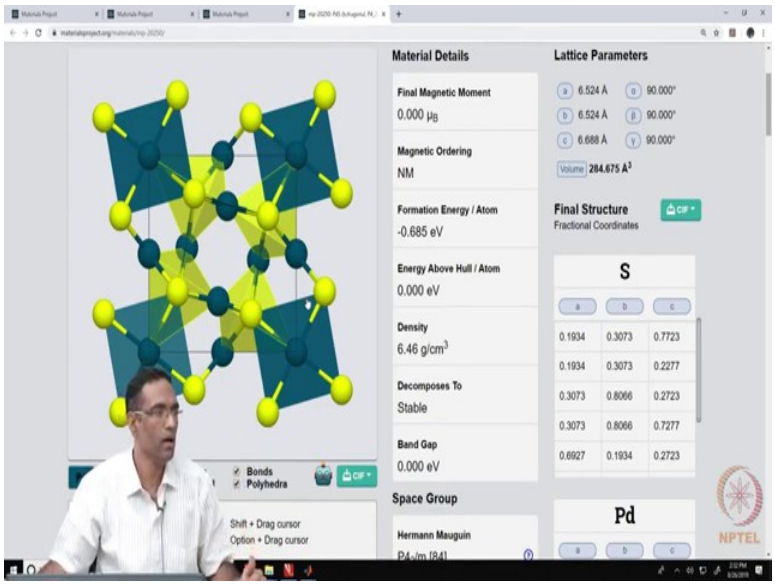
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Decomposes To
Stable
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Hermann Mauguin
$P4_2/m$ (84)
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Volume 284.675 Å^3
Final Structure
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S
a b c
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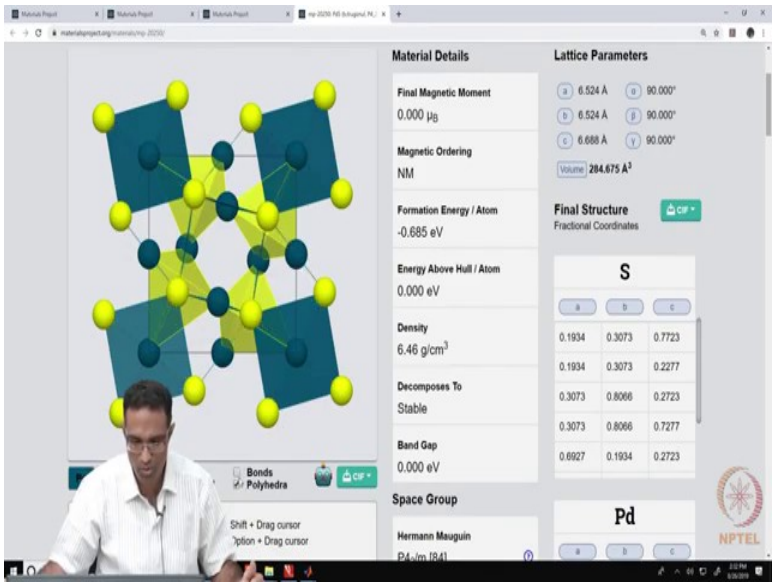
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Decomposes To
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Band Gap
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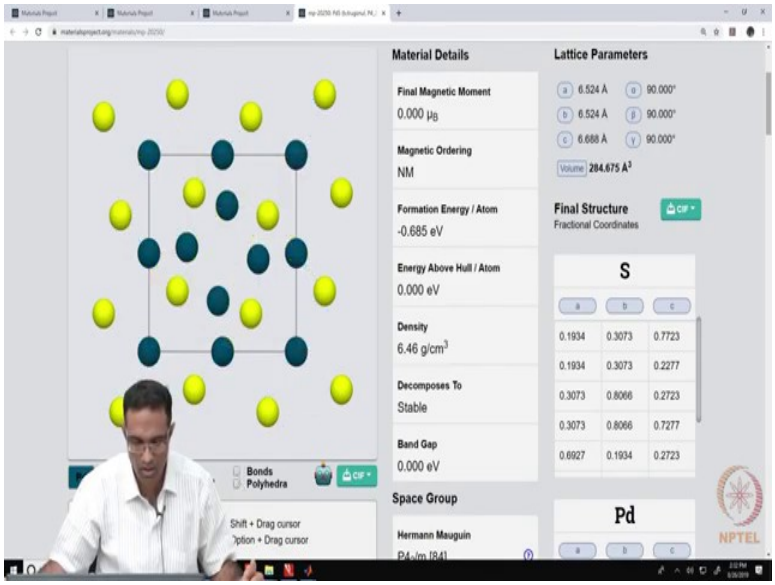
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CIF
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a b c
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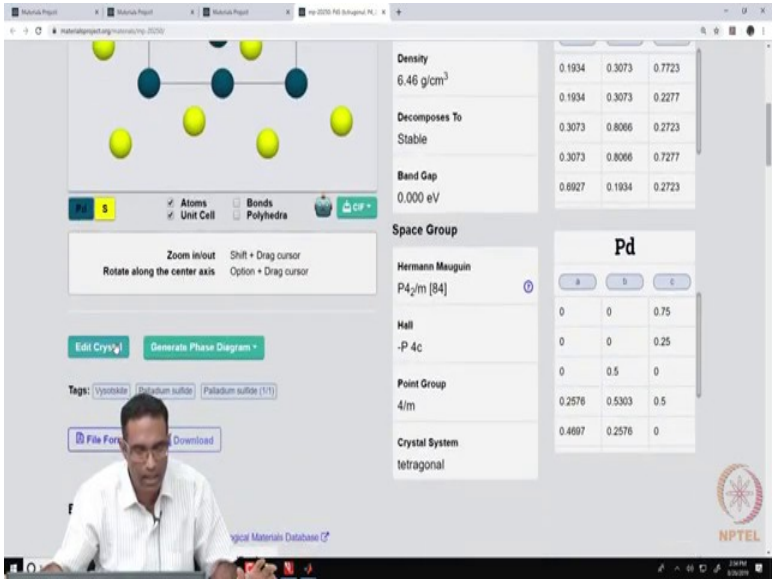
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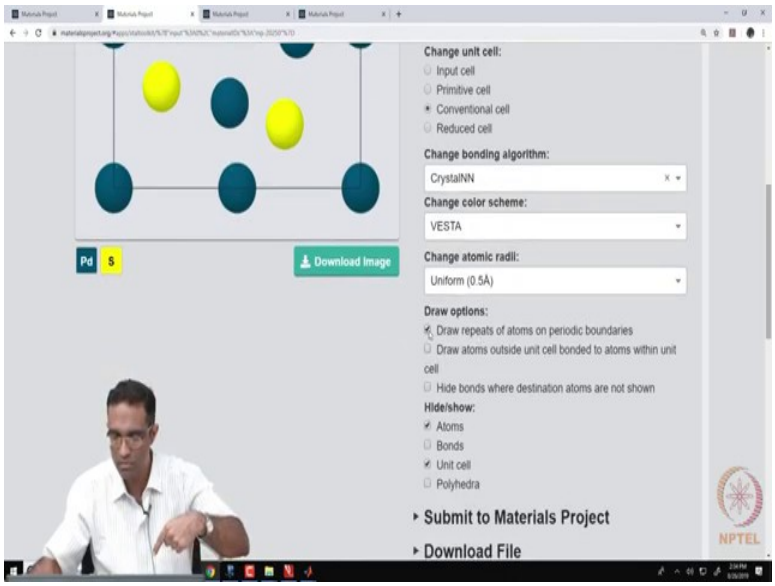
Pd
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Download Image
Change unit cell:
Input cell
Primitive cell
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Change bonding algorithm:
CrystalNN
Change color scheme:
VESTA
Change atomic radii:
Uniform (0.5Å)
Draw options:
Draw repeats of atoms on periodic boundaries
Draw atoms outside unit cell bonded to atoms within unit cell
Hide bonds where destination atoms are not shown
Hide/show:
Atoms
Bonds
Unit cell
Polyhedra
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So, now let us look at some example that we are probably going to be creating in class now. I am going to choose an example of palladium sulfite, palladium sulfite and I am interested in regenerating the, this particular structure right here with P4 2 over m, which is tetragonal once again. So I click on that.

And it gives me the corresponding visualization of the structure. So, when you generate it using the MATLAB code I am going to be giving you. You should also be able to check whether what you are doing is correct or wrong by going to this website, any arbitrary compound.

And this website is fairly simple to use. We do not want to show bonds, we do not want to show polyhedra, we just want to show the atoms at the unit. So, this is how it looks. Now, if you look at the lattice parameters on the right hand side part of the website right here you have A, B and C and alpha, beta, gamma as 90 degrees. Sometimes it so happens that for centered lattices, they use a primitive lattice vector. They use a primitive lattice vector.

When they use a primitive lattice vector, you will see A, B and C, but you will see alpha, beta, gamma being different from what you were expecting. For example, if they use face centered for face centered lattices, if they are using a primitive lattice vector, you will not see alpha, beta, gamma to be 90 degrees, only for non-primitive lattice vectors is alpha, beta gamma 90 degrees for the face centered cubic structure.

In that case, if you are encountering that situation, and if you want to still view it in the standard setting, that means you want to view it with the non-primitive lattice vectors. What you do is, you go down in this website and click Edit crystal. Once you click Edit crystal, the website takes some time to load something called as the crystal toolkit.

These things are very simple to use and extremely useful. And I already have the page open right here. So, this is what happened. This is what opens up. This is what opens up and you can choose on the right hand side, what type of cell that you want, cell you want to generate. So, I click conventional cell which means that A be it is not primitive, it is basically not primitive. So, now you see and you have the legends which is indicating you where palladium is located and where sulfur is located.

And sometimes what happens is you get a palladium atom here, you also get a palladium atom here, but that is occurring because of lattice translations. And you can check this off and wait for some time.

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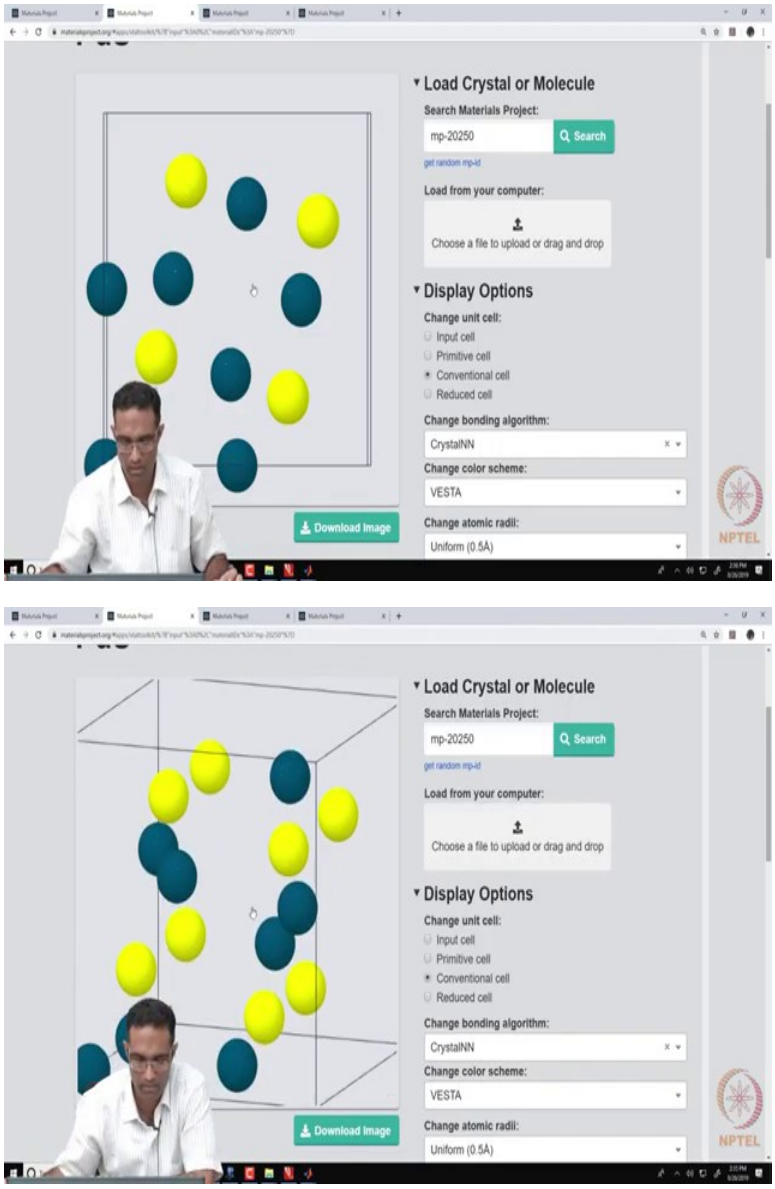

And you will see that the atoms that are there on the other on the edges basically disappear. So, this is actually the unit cell. And you can rotate it and take a look at it. Now, we are going to generate this palladium sulfide or palladium sulfide PdS molecule with our MATLAB code, we are going to generate only one unit cell.

So, there is a significant modification that was that I have done to the MATLAB code so that you will be able to view only the atoms belonging to that particular unit cell. It is quite simple for cubic systems to add to those few lines of code. But once the unit cell is not cubic, it is like mono clinic and stuff like that you have to do a little bit of cut of analytical geometry to actually see how you can store atoms which only belong inside that particular unit cell.